

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sseptal617srh

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\*\*\*\*\* Welcome to STN International \*\*\*\*\*

NEWS 1 Web Page for STN Seminar Schedule - N. America  
NEWS 2 DEC 01 ChemPort single article sales feature unavailable  
NEWS 3 APR 03 CAS coverage of exemplified prophetic substances enhanced  
NEWS 4 APR 07 STN is raising the limits on saved answers  
NEWS 5 APR 24 CA/CAPLUS now has more comprehensive patent assignee information  
NEWS 6 APR 26 USPATFULL and USPAT2 enhanced with patent assignment/reassignment information  
NEWS 7 APR 28 CAS patent authority coverage expanded  
NEWS 8 APR 28 ENCOMPLIT/ENCOMPLIT2 search fields enhanced  
NEWS 9 APR 28 Limits doubled for structure searching in CAS REGISTRY  
NEWS 10 MAY 08 STN Express, Version 8.4, now available  
NEWS 11 MAY 11 STN on the Web enhanced  
NEWS 12 MAY 11 BEILSTEIN substance information now available on STN Easy  
NEWS 13 MAY 14 DGENE, PCTGEN and USGENE enhanced with increased limits for exact sequence match searches and introduction of free HIT display format  
NEWS 14 MAY 15 INPADOCDB and INPAFAMDB enhanced with Chinese legal status data  
NEWS 15 MAY 28 CAS databases on STN enhanced with NANO super role in records back to 1992  
NEWS 16 JUN 01 CAS REGISTRY Source of Registration (SR) searching enhanced on STN  
NEWS 17 JUN 26 NUTRACEUT and PHARMAML no longer updated  
NEWS 18 JUN 29 IMSCOPROFILE now reloaded monthly  
NEWS 19 JUN 29 EFFULL adds Simultaneous Left and Right Truncation (SLART) to AB, MCLM, and TI fields  
NEWS 20 JUL 09 PATDPAFULL adds Simultaneous Left and Right Truncation (SLART) to AB, CLM, MCLM, and TI fields  
NEWS 21 JUL 14 USGENE enhances coverage of patent sequence location (PSL) data  
NEWS 22 JUL 27 CA/CAPLUS enhanced with new citing references  
NEWS 23 JUL 16 GBFULL adds patent backfile data to 1855  
NEWS 24 JUL 21 USGENE adds bibliographic and sequence information  
NEWS 25 JUL 28 EFFULL adds first-page images and applicant-cited references  
NEWS 26 JUL 28 INPADOCDB and INPAFAMDB add Russian legal status data  
NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,  
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS LOGIN Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 09:38:52 ON 29 JUL 2009

=> fil reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.44	0.44

FILE 'REGISTRY' ENTERED AT 09:39:58 ON 29 JUL 2009  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2009 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 27 JUL 2009 HIGHEST RN 1169753-75-6  
DICTIONARY FILE UPDATES: 27 JUL 2009 HIGHEST RN 1169753-75-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

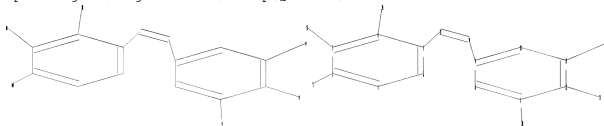
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\10-790662.str



```

chain nodes :
13 14 15 16 17 18 19 20
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
2-17 3-16 4-15 5-13 7-20 9-14 11-19 12-18 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
3-16 4-15
exact bonds :
2-17 5-13 7-20 9-14 11-19 12-18 13-14
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

```

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS

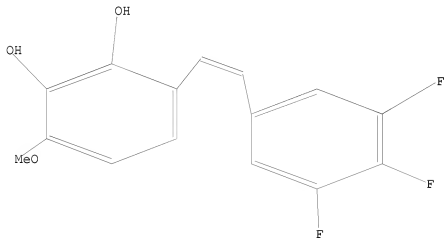
```

L1 STRUCTURE UPLOADED

```

=> d
L1 HAS NO ANSWERS
L1 STR

```

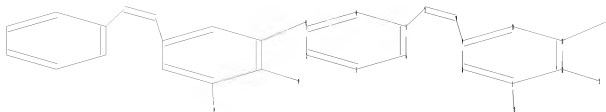


Structure attributes must be viewed using STN Express query preparation.

```

=>
Uploading C:\Program Files\Stnexp\Queries\10-790662 a.str

```



```

chain nodes :
13 14 15 16 17
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
5-13 7-17 9-14 11-16 12-15 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact bonds :
5-13 7-17 9-14 11-16 12-15 13-14
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

```

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS

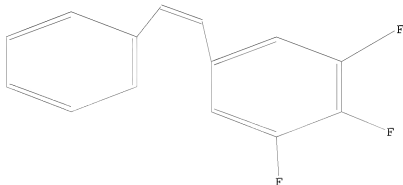
```

L2 STRUCTURE UPLOADED

```

=> d
L2 HAS NO ANSWERS
L2 STR

```



Structure attributes must be viewed using STN Express query preparation.

```

=> s 12
SAMPLE SEARCH INITIATED 09:43:25 FILE 'REGISTRY'

```

SAMPLE SCREEN SEARCH COMPLETED - 62 TO ITERATE

100.0% PROCESSED 62 ITERATIONS 8 ANSWERS  
SEARCH TIME: 00.00.01

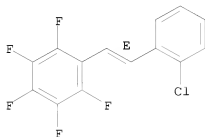
FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 768 TO 1712  
PROJECTED ANSWERS: 8 TO 329

L3 8 SEA SSS SAM L2

=> d scan

L3 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, [(1E)-2-(2-chlorophenyl)ethenyl]pentafluoro- (9CI)  
MF C14 H6 Cl F5

Double bond geometry as shown.

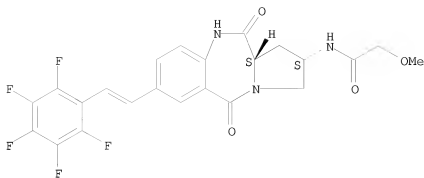


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):7

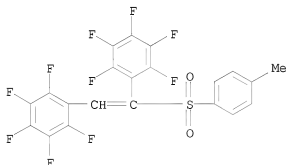
L3 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Acetamide, N-[(2S,11aS)-2,3,5,10,11,11a-hexahydro-5,11-dioxo-7-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-1H-pyrrolo[2,1-c][1,4]benzodiazepin-2-yl]-2-methoxy-  
MF C23 H18 F5 N3 O4

Absolute stereochemistry.  
Double bond geometry unknown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

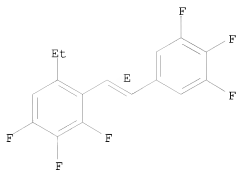
L3 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-[1-[(4-methylphenyl)sulfonyl]-1,2-ethenediyl]bis[2,3,4,5,6-  
 pentafluoro- (9CI)  
 MF C21 H8 F10 O2 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1-ethyl-3,4,5-trifluoro-2-[(1E)-2-(3,4,5-trifluorophenyl)ethenyl]-  
 MF C16 H10 F6

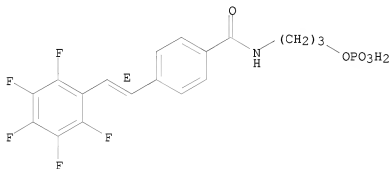
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

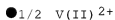
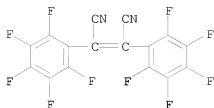
L3 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzamide, 4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-N-[3-(  
 phosphonooxy)propyl]-  
 MF C18 H15 F5 N O5 P

Double bond geometry as shown.



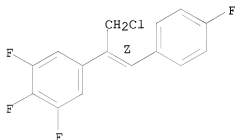
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 2-Butenedinitrile, 2,3-bis(pentafluorophenyl)-, radical ion(1-),  
 vanadium(2+), (2E)- (9CI)  
 MF C16 F10 N2 . 1/2 V  
 CI COM, RIS



L3 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 5-[(1Z)-1-(chloromethyl)-2-(4-fluorophenyl)ethenyl]-1,2,3-  
 trifluoro-  
 MF C15 H9 Cl F4

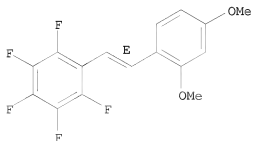
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 8 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1-[(1E)-2-(2,4-dimethoxyphenyl)ethenyl]-2,3,4,5,6-pentafluoro-  
 MF C16 H11 F5 O2

Double bond geometry as shown.





\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> s 12 full

FULL SEARCH INITIATED 09:48:03 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1496 TO ITERATE

100.0% PROCESSED 1496 ITERATIONS

201 ANSWERS

SEARCH TIME: 00.00.01

L4 201 SEA SSS FUL L2

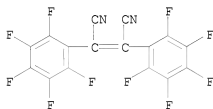
=> d scan

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN 2-Butenedinitrile, 2,3-bis(pentafluorophenyl)-, radical ion(1-), (2E)-(9CI)

MF C16 F10 N2

CI COM, RIS



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):200\  
'200\' IS NOT VALID HERE

To display more answers, enter the number of answers you would like to see. To end the display, enter "NONE", "N", "0", or "END".

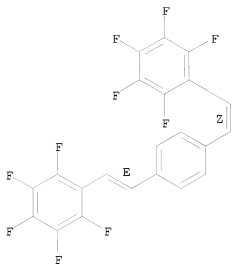
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):200

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-

MF C22 H8 F10

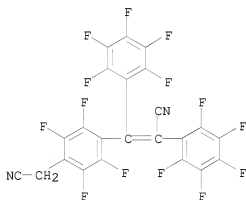
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile,  $\alpha$ -[4-(cyanomethyl)-2,3,5,6-tetrafluorophenyl] (2,3,4,5,6-pentafluorophenyl)methylenel-2,3,4,5,6-pentafluoro-, compd. with cyclohexanamine (1:1)  
 MF C23 H2 F14 N2 . C6 H13 N

CM 1



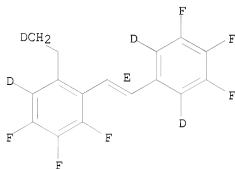
CM 2



L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene-1,3-d2, 2-[(1E)-2-[2-(ethyl-2-d)-4,5,6-trifluorophenyl-3-d]ethenyl]-4,5,6-trifluoro-  
MF C16 H6 D4 F6

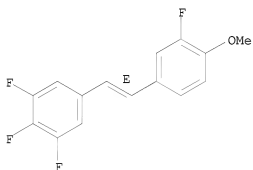
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, 1,2,3-trifluoro-5-[(1E)-2-(3-fluoro-4-methoxyphenyl)ethenyl]-  
MF C15 H10 F4 O

Double bond geometry as shown.

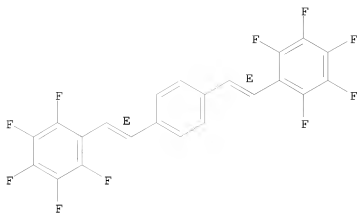


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, 1,2-dimethyl-, compd. with  
(E,E)-1,4-bis[2-(pentafluorophenyl)ethenyl]benzene (1:1) (9CI)  
MF C22 H8 F10 . C8 H10

CM 1

Double bond geometry as shown.

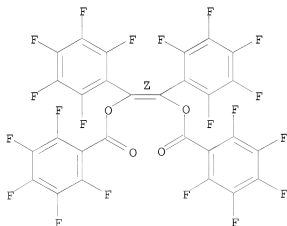


CM 2



L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzoic acid, pentafluoro-, 1,2-bis(pentafluorophenyl)-1,2-ethenediyl  
 ester, (Z)- (9CI)  
 MF C28 F20 O4

Double bond geometry as shown.

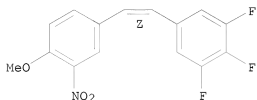


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3-trifluoro-5-[(1Z)-2-(4-methoxy-3-nitrophenyl)ethenyl]-  
MF C15 H10 F3 N O3

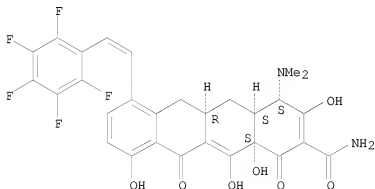
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

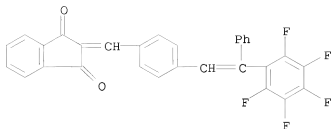
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-  
3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[2-(2,3,4,5,6-  
pentafluorophenyl)ethenyl]-, (4S,4aS,5aR,12aS)-  
MF C29 H23 F5 N2 O7

Absolute stereochemistry.  
Double bond geometry unknown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

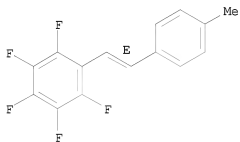
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 1H-indene-1,3(2H)-dione, 2-[[4-[2-(2,3,4,5,6-pentafluorophenyl)-2-  
phenylethenyl]phenyl]methylene]-  
MF C30 H15 F5 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, pentafluoro[(1E)-2-(4-methylphenyl)ethenyl]- (9CI)  
 MF C15 H9 F5

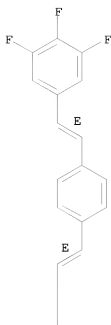
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Bicyclo[2.2.2]octane, 1-bromo-4-[(1E)-2-[4-[(1E)-2-(3,4,5-trifluorophenyl)ethenyl]phenyl]ethenyl]-  
 MF C24 H22 Br F3

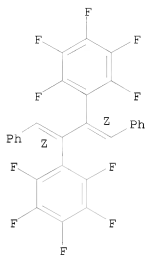
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

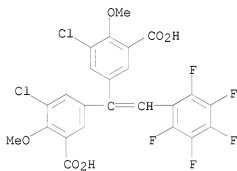
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-[(1Z,2Z)-1,2-bis(phenylmethylene)-1,2-  
 ethanediyl]bis[2,3,4,5,6-pentafluoro- (9CI)  
 MF C28 H12 F10

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

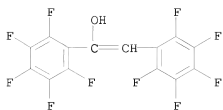
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzoic acid, 3,3'-[(pentafluorophenyl)ethenylidene]bis[5-chloro-6-methoxy-  
 (9CI)  
 MF C24 H13 Cl2 F5 O6  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenemethanol, 2,3,4,5,6-pentafluoro- $\alpha$ -[(2,3,4,5,6-pentafluorophenyl)methylene]-, sodium salt (1:1)  
 MF C14 H2 F10 O . Na

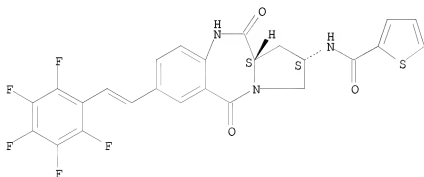




\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 2-Thiophenecarboxamide, N-[(2S,11aS)-2,3,5,10,11,11a-hexahydro-5,11-dioxo-7-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-1H-pyrrolo[2,1-c][1,4]benzodiazepin-2-yl]-  
 MF C25 H16 F5 N3 O3 S

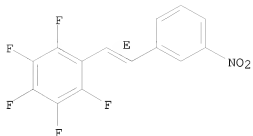
Absolute stereochemistry.  
 Double bond geometry unknown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

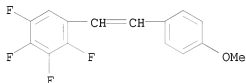
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-(3-nitrophenyl)ethenyl]-  
 MF C14 H6 F5 N O2

Double bond geometry as shown.



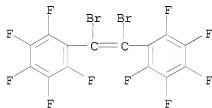
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3,4-tetrafluoro-5-[2-(4-methoxyphenyl)ethenyl]-  
 MF C15 H10 F4 O



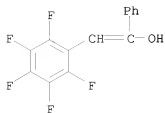
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-(1,2-dibromo-1,2-ethenediyl)bis[2,3,4,5,6-pentafluoro-  
 MF C14 Br2 F10



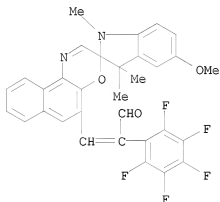
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenemethanol, α-[(2,3,4,5,6-pentafluorophenyl)methylene]-  
 MF C14 H7 F5 O  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

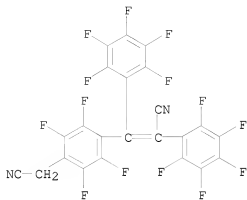
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetaldehyde,  $\alpha$ -[(1,3-dihydro-5-methoxy-1,3,3-trimethylspiro[2H-indole-2,3'-[3H]naphth[2,1-b][1,4]oxazin]-5'-yl)methylene]-2,3,4,5,6-pentafluoro-  
 MF C23 H23 F5 N2 O3



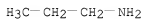
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile,  $\alpha$ -[[4-(cyanomethyl)-2,3,5,6-tetrafluorophenyl](2,3,4,5,6-pentafluorophenyl)methylene]-2,3,4,5,6-pentafluoro-, compd. with 1-propanamine (1:1)  
 MF C23 H2 F14 N2 . C3 H9 N

CM 1



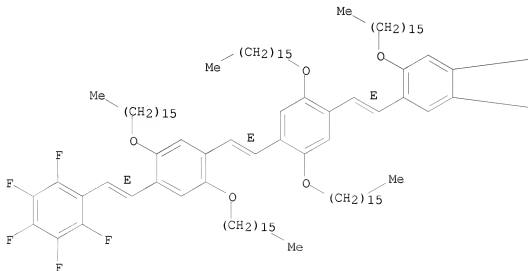
CM 2

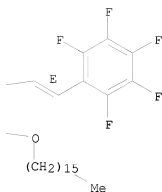


L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,4-bis[(1E)-2-[2,5-bis(hexadecyloxy)-4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]phenyl]ethenyl]-2,5-bis(hexadecyloxy)-  
 MF C134 H212 F10 O6

Double bond geometry as shown.

PAGE 1-A

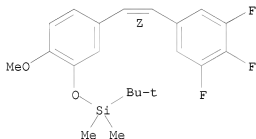




\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 5-[(1Z)-2-{3-[(1,1-dimethylethyl)dimethylsilyl]oxy}-4-  
 methoxyphenyl]ethenyl]-1,2,3-trifluoro-  
 MF C21 H25 F3 O2 Si

Double bond geometry as shown.

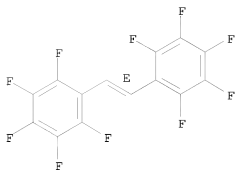


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-(1,2-ethenediyl)bis[2,3,4,5,6-pentafluoro-, (E)-, compd.  
 with (E)-1,1'-(1,2-ethenediyl)bis[benzene] (1:1) (9CI)  
 MF C14 H12 . C14 H2 F10

CM 1

Double bond geometry as shown.



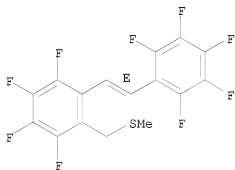
CM 2

Double bond geometry as shown.



L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, pentafluoro[2-[2,3,4,5-tetrafluoro-6-  
 [(methylthio)methyl]phenyl]ethenyl]-, (E)- (9CI)  
 MF C16 H7 F9 S

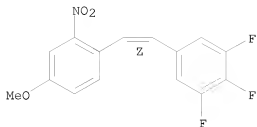
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

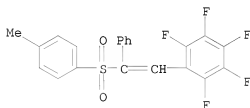
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3-trifluoro-5-[(1Z)-2-(4-methoxy-2-nitrophenyl)ethenyl]-  
 MF C15 H10 F3 N O3

Double bond geometry as shown.



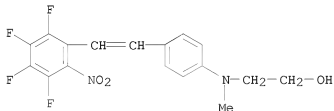
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3,4,5-pentafluoro-6-[2-[(4-methylphenyl)sulfonyl]-2-phenylethenyl]-  
 MF C21 H13 F5 O2 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

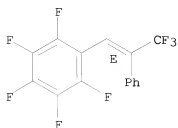
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Ethanol, 2-[methyl[4-[2-(2,3,4,5-tetrafluoro-6-nitrophenyl)ethenyl]phenyl]amino]-  
 MF C17 H14 F4 N2 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, pentafluoro(3,3,3-trifluoro-2-phenyl-1-propenyl)-, (E)- (9CI)  
 MF C15 H6 F8

Double bond geometry as shown.

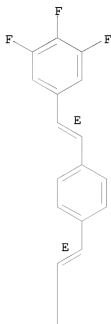


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Bicyclo[2.2.2]octane, 1-methoxy-4-[(1E)-2-[4-[(1E)-2-(3,4,5-  
trifluorophenyl)ethenyl]phenyl]ethenyl]-  
MF C25 H25 F3 O

Double bond geometry as shown.

PAGE 1-A

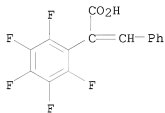






\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

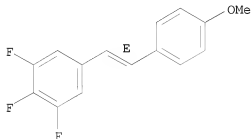
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenecetic acid, 2,3,4,5,6-pentafluoro- $\alpha$ -(phenylmethylene)-  
 MF C15 H7 F5 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3-trifluoro-5-[(1E)-2-(4-methoxyphenyl)ethenyl]-  
 MF C15 H11 F3 O

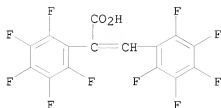
Double bond geometry as shown.



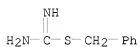
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenecetic acid, 2,3,4,5,6-pentafluoro- $\alpha$ -[(2,3,4,5,6-pentafluorophenyl)methylene]-, compd. with phenylmethyl carbamimidothioate  
 (1:1)  
 MF C15 H2 F10 O2 . C8 H10 N2 S

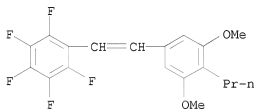
CM 1



CM 2



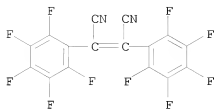
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1-[2-(3,5-dimethoxy-4-propylphenyl)ethenyl]-2,3,4,5,6-pentafluoro-  
 MF C19 H17 F5 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 2-Butenedinitrile, 2,3-bis(pentafluorophenyl)-, radical ion(1-),  
 vanadium(2+), (2E)-, compd. with tetrahydrofuran (9CI)  
 MF C16 F10 N2 . x C4 H8 O . 1/2 V

CM 1

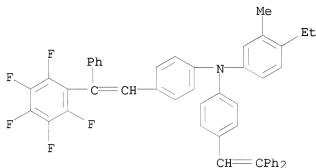


● 1/2 V(II) 2+

CM 2



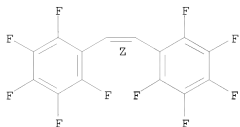
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenamine, N-[4-(2,2-diphenylethenyl)phenyl]-4-ethyl-3-methyl-N-[4-(2-  
 (2,3,4,5,6-pentafluorophenyl)-2-phenylethenyl)phenyl]-  
 MF C49 H36 F5 N



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

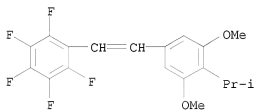
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-(1Z)-1,2-ethenediylbis[2,3,4,5,6-pentafluoro- (9CI)  
 MF C14 H2 F10

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

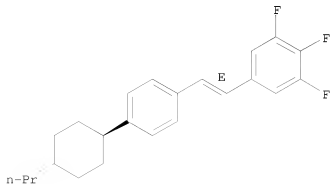
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1-[2-[3,5-dimethoxy-4-(1-methylethyl)phenyl]ethenyl]-2,3,4,5,6-  
 pentafluoro-  
 MF C19 H17 F5 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3-trifluoro-5-[(1E)-2-[4-(trans-4-  
 propylcyclohexyl)phenyl]ethenyl]-  
 MF C23 H25 F3

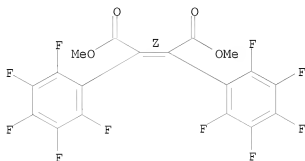
Relative stereochemistry.  
 Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

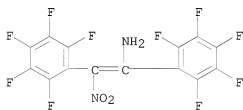
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 2-Butenedioic acid, 2,3-bis(pentafluorophenyl)-, dimethyl ester, (Z)-  
(9CI)  
MF C18 H6 F10 O4

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

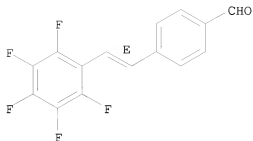
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzenemethanamine, 2,3,4,5,6-pentafluoro- $\alpha$ -(nitro(2,3,4,5,6-pentafluorophenyl)methylene)-  
MF C14 H2 F10 N2 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzaldehyde, 4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-  
MF C15 H7 F5 O

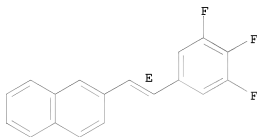
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Naphthalene, 2-[(1E)-2-(3,4,5-trifluorophenyl)ethenyl]-  
 MF C18 H11 F3

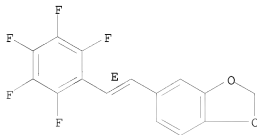
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 1,3-Benzodioxole, 5-[2-(pentafluorophenyl)ethenyl]-, (E)- (9CI)  
 MF C15 H7 F5 O2

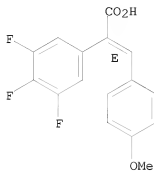
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

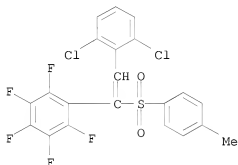
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenecacetic acid, 3,4,5-trifluoro- $\alpha$ -[(4-methoxyphenyl)methylene]-,  
 (αE)-  
 MF C16 H11 F3 O3

Double bond geometry as shown.



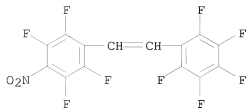
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1-[2-(2,6-dichlorophenyl)-1-[(4-methylphenyl)sulfonyl]ethenyl]-  
 2,3,4,5,6-pentafluoro-  
 MF C21 H11 Cl2 F5 O2 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

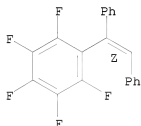
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, pentafluoro[2-(2,3,5,6-tetrafluoro-4-nitrophenyl)ethenyl]- (9CI)  
 MF C14 H2 F9 N O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

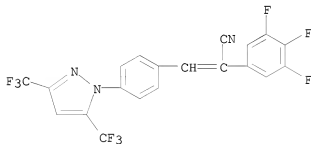
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, [(1Z)-(1,2-diphenylethenyl)]pentafluoro- (9CI)  
 MF C20 H11 F5

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile, α-[[4-[3,5-bis(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]methylene]-3,4,5-trifluoro-  
 MF C20 H8 F9 N3



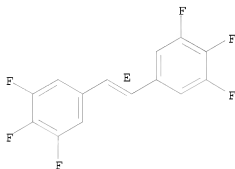
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-(1E)-1,2-ethenediylbis[3,4,5-trifluoro- (9CI)



MF C14 H6 F6

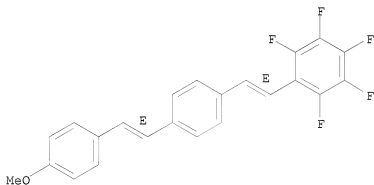
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, 1-[2-(4-methoxyphenyl)ethenyl]-4-[2-(pentafluorophenyl)ethenyl]-,  
(E,E)- (9CI)  
MF C23 H15 F5 O

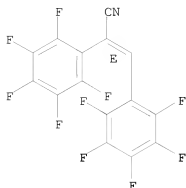
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Acrylonitrile, 2,3-bis(pentafluorophenyl)-, (E)- (8CI)  
MF C15 H F10 N

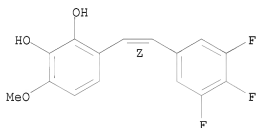
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 1,2-Benzenediol, 3-methoxy-6-[(1Z)-2-(3,4,5-trifluorophenyl)ethenyl]-  
 MF C15 H11 F3 O3

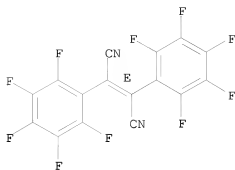
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

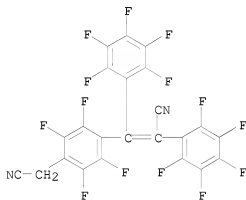
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 2-Butenedinitrile, 2,3-bis(pentafluorophenyl)-, (2E)- (9CI)  
 MF C16 F10 N2

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

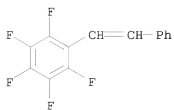
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile,  $\alpha$ -[[4-(cyanomethyl)-2,3,5,6-tetrafluorophenyl](2,3,4,5,6-pentafluorophenyl)methylene]-2,3,4,5,6-pentafluoro-, compd. with N,N-diethylethanamine (1:1)  
 MF C23 H2 F14 N2 . C6 H15 N  
 CM 1



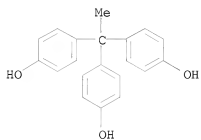
CM 2



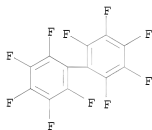
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN INDEX NAME NOT YET ASSIGNED  
 MF (C20 H18 O3 . C14 H7 F5 . C12 F10)x  
 CI PMS  
 CM 1



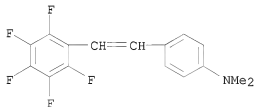
CM 2



CM 3



L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenamine, N,N-dimethyl-4-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-  
 MF C16 H12 F5 N

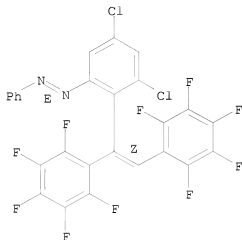


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Diazene, 1-[2-[(1Z)-1,2-bis(2,3,4,5,6-pentafluorophenyl)ethenyl]-3,5-dichlorophenyl]-2-phenyl-, (1E)-  
 MF C26 H8 Cl2 F10 N2

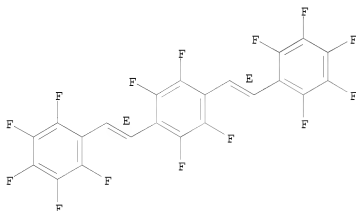
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,4,5-tetrafluoro-3,6-bis[2-(pentafluorophenyl)ethenyl]-,  
 (E,E)- (9CI)  
 MF C22 H4 F14

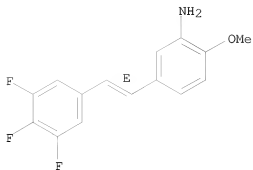
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenamine, 2-methoxy-5-[(1E)-2-(3,4,5-trifluorophenyl)ethenyl]-  
 MF C15 H12 F3 N O

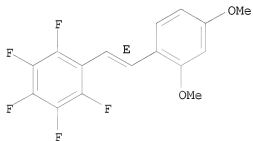
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

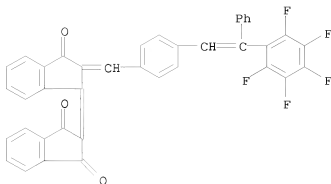
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1-[(1E)-2-(2,4-dimethoxyphenyl)ethenyl]-2,3,4,5,6-pentafluoro-  
 MF C16 H11 F5 O2

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

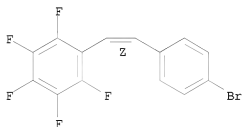
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 1H-Indene-1,3(2H)-dione, 2-[2,3-dihydro-3-oxo-2-[[4-[2-(2,3,4,5,6-pentafluorophenyl)-2-phenylethenyl]phenyl]methylene]-1H-inden-1-ylidene]-  
 MF C39 H19 F5 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, [2-(4-bromophenyl)ethenyl]pentafluoro-, (Z)- (9CI)  
 MF C14 H6 Br F5

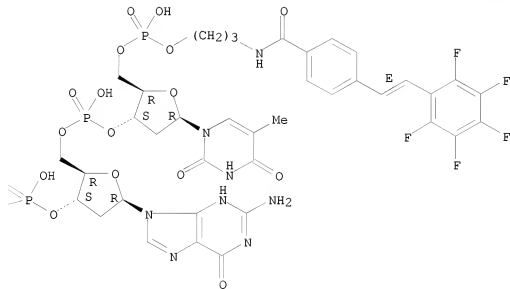
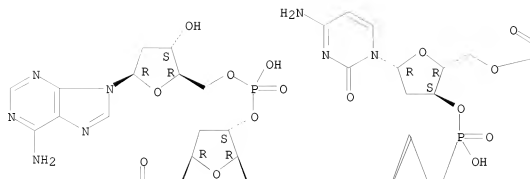
Double bond geometry as shown.



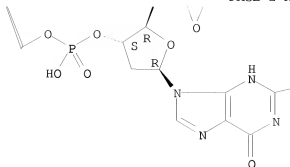
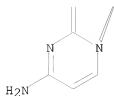
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Adenosine, 5'-O-[hydroxy[3-[[4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]benzoyl]amino]propoxy]phosphinyl]thymidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxy-  
 MF C76 H87 F5 N24 O38 P6

Absolute stereochemistry.  
 Double bond geometry as shown.







PAGE 2-A

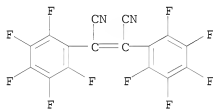
PAGE 2-B

NH<sub>2</sub>

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 2-Butenedinitrile, 2,3-bis(pentafluorophenyl)-, radical ion(1-),  
 vanadium(2+), (2E)-, compd. with acetonitrile (9CI)  
 MF C16 F10 N2 . x C2 H3 N . 1/2 V

CM 1



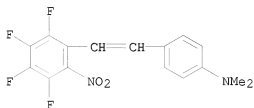
● 1/2 V(II) 2+

CM 2



L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzenamine, N,N-dimethyl-4-[2-(2,3,4,5-tetrafluoro-6-nitrophenyl)ethenyl]-  
MF C16 H12 F4 N2 O2

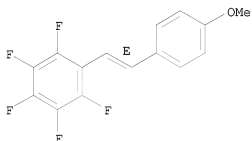


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-(4-methoxyphenyl)ethenyl]-  
MF C15 H9 F5 O

Double bond geometry as shown.



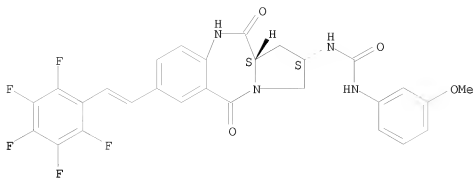
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Urea, N-[(2S,11aS)-2,3,5,10,11,11a-hexahydro-5,11-dioxo-7-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-1H-pyrrolo[2,1-c][1,4]benzodiazepin-2-yl]-N'-(3-methoxyphenyl)-  
MF C28 H21 F5 N4 O4

Absolute stereochemistry.

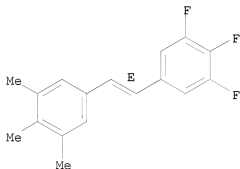
Double bond geometry unknown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3-trifluoro-5-[(1E)-2-(3,4,5-trimethylphenyl)ethenyl]-  
 MF C17 H15 F3

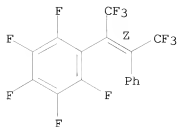
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, pentafluoro[3,3,3-trifluoro-2-phenyl-1-(trifluoromethyl)-1-propenyl]-, (Z)- (9CI)  
 MF C16 H5 F11

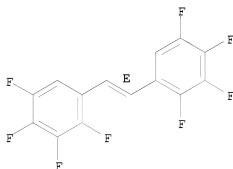
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

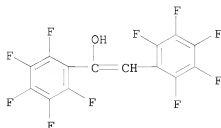
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-(1,2-ethenediyl)bis[2,3,4,5-tetrafluoro-, (E)- (9CI)  
 MF C14 H4 F8

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

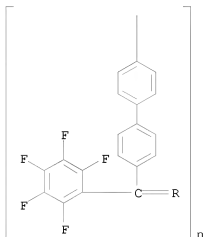
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenemethanol, 2,3,4,5,6-pentafluoro- $\alpha$ -[(2,3,4,5,6-pentafluorophenyl)methylene]-  
 MF C14 H2 F10 O  
 CI COM



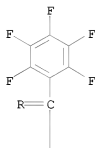
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Poly[[1,1'-biphenyl]-4,4'-diyl[(1Z)-1,2-bis(pentafluorophenyl)-1,2-ethenediyl]] (9CI)  
 MF (C26 H8 F10)n  
 CI PMS

PAGE 1-A

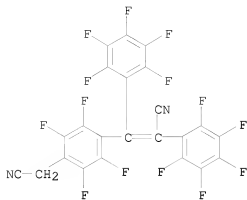


PAGE 2-A



L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile,  $\alpha$ -[[4-(cyanomethyl)-2,3,5,6-tetrafluorophenyl](2,3,4,5,6-pentafluorophenyl)methylene]-2,3,4,5,6-pentafluoro-, compd. with N-(1-methylethyl)-2-propanamine (1:1)  
 MF C23 H2 F14 N2 . C6 H15 N

CM 1

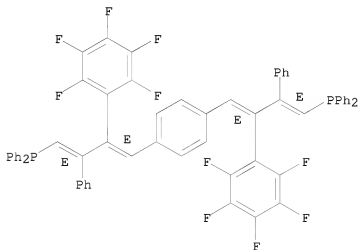


CM 2

i-Pr-NH-Pr-i

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Phosphine, 1,1'-[1,4-phenylenebis(1E,3E)-3-(2,3,4,5,6-pentafluorophenyl)-  
 4-phenyl-1,3-butadiene-4,1-diyl]]bis[1,1-diphenyl-  
 MF C62 H38 F10 P2

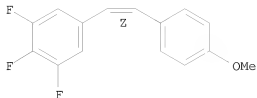
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3-trifluoro-5-[(1Z)-2-(4-methoxyphenyl)ethenyl]-  
 MF C15 H11 F3 O

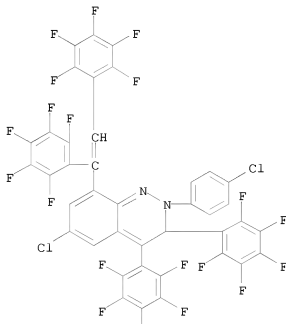
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Cinnoline, 8-[1,2-bis(2,3,4,5,6-pentafluorophenyl)ethenyl]-6-chloro-2-(4-  
 chlorophenyl)-2,3-dihydro-3,4-bis(2,3,4,5,6-pentafluorophenyl)-  
 MF C40 H8 Cl2 F20 N2

PAGE 1-A



PAGE 2-A

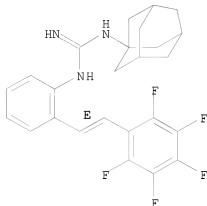


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Guanidine, N-[2-[2-(pentafluorophenyl)ethenyl]phenyl]-N'-

tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl-, monohydrochloride, (E)- (9CI)  
 MF C25 H24 F5 N3 . Cl H

Double bond geometry as shown.

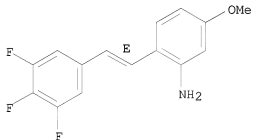


● HCl

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenamine, 5-methoxy-2-[(1E)-2-(3,4,5-trifluorophenyl)ethenyl]-  
 MF C15 H12 F3 N O

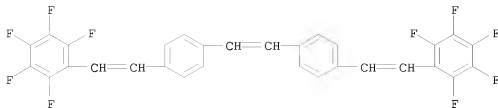
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

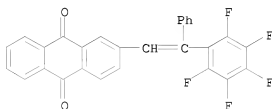
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-(1,2-ethenediyl)bis[4-[2-(pentafluorophenyl)ethenyl]- (9CI)  
 MF C30 H14 F10





\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

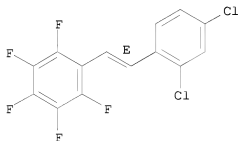
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 9,10-Anthracenedione, 2-[2-(2,3,4,5,6-pentafluorophenyl)-2-phenylethenyl]-  
 MF C28 H13 F5 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, [2-(2,4-dichlorophenyl)ethenyl]pentafluoro-, (E)- (9CI)  
 MF C14 H5 Cl2 F5

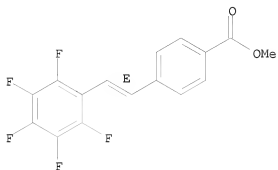
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

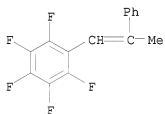
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzoic acid, 4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-, methyl  
 ester  
 MF C16 H9 F5 O2

Double bond geometry as shown.



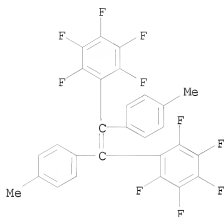
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3,4,5-pentafluoro-6-(2-phenyl-1-propen-1-yl)-  
 MF C15 H9 F5



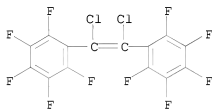
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-[1,2-bis(4-methylphenyl)-1,2-ethenediyl]bis[2,3,4,5,6-  
 pentafluoro-  
 MF C28 H14 F10



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

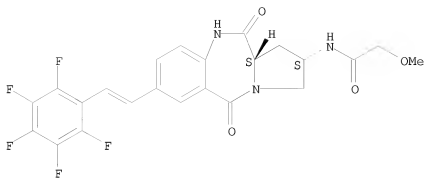
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-(1,2-dichloro-1,2-ethenediyl)bis[2,3,4,5,6-pentafluoro-  
 MF C14 C12 F10



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Acetamide, N-[(2S,11aS)-2,3,5,10,11,11a-hexahydro-5,11-dioxo-7-[(2-  
 (2,3,4,5,6-pentafluorophenyl)ethenyl)-1H-pyrrolo[2,1-c][1,4]benzodiazepin-  
 2-yl]-2-methoxy-  
 MF C23 H18 F5 N3 O4

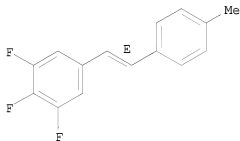
Absolute stereochemistry.  
 Double bond geometry unknown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3-trifluoro-5-[(1E)-2-(4-methylphenyl)ethenyl]-  
 MF C15 H11 F3

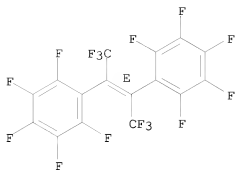
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

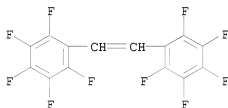
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-[1,2-bis(trifluoromethyl)-1,2-ethenediyl]bis[2,3,4,5,6-  
 pentafluoro-, (E)- (9CI)  
 MF C16 F16

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

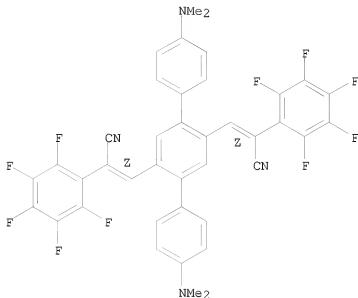
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-(1,2-ethenediyl)bis[2,3,4,5,6-pentafluoro-  
 MF C14 H2 F10



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

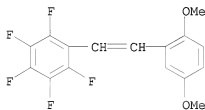
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile,  $\alpha,\alpha'$ -[[4,4''-  
 bis(dimethylamino)[1,1':4',1''-terphenyl]-2',5'-  
 diyl]dimethyldiynyl]bis[2,3,4,5,6-pentafluoro-, ( $\alpha$ Z, $\alpha'$ Z)- (9CI)  
 MF C40 H24 F10 N4

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

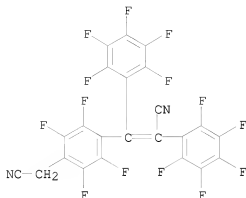
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1-[2-(2,5-dimethoxyphenyl)ethenyl]-2,3,4,5,6-pentafluoro-  
 MF C16 H11 F5 O2



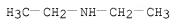
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile,  $\alpha$ -[[4-(cyanomethyl)-2,3,5,6-tetrafluorophenyl](2,3,4,5,6-pentafluorophenyl)methylene]-2,3,4,5,6-pentafluoro-, compd. with N-ethylethanamine (1:1)  
 MF C23 H2 F14 N2 . C4 H11 N

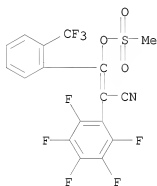
CM 1



CM 2



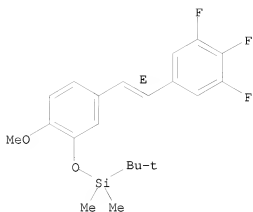
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile, 2,3,4,5,6-pentafluoro- $\alpha$ -  
 [[methylsulfonyl]oxy][2-(trifluoromethyl)phenyl]methylene]-  
 MF C17 H7 F8 N O3 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 5-[(1E)-2-{3-[[1,1-dimethylethyl]dimethylsilyl]oxy}-4-  
 methoxyphenyl]ethenyl]-1,2,3-trifluoro-  
 MF C21 H25 F3 O2 Si

Double bond geometry as shown.

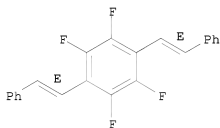


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,4,5-tetrafluoro-3,6-bis(2-phenylethenyl)-, (E,E)-, polymer  
 with (E,E)-1,4-bis[2-(pentafluorophenyl)ethenyl]benzene (9CI)  
 MF (C22 H14 F4 . C22 H8 F10)x  
 CI PMS

CM 1

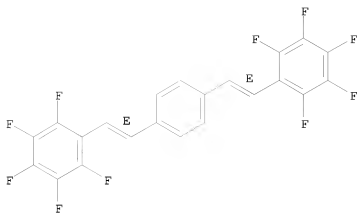
Double bond geometry as shown.



CM 2

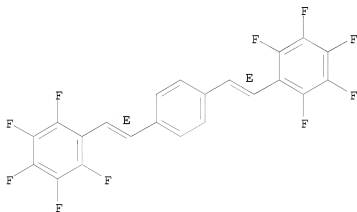
Double bond geometry as shown.





L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,4-bis[(1E)-2-(pentafluorophenyl)ethenyl]- (9CI)  
 MF C22 H8 F10  
 CI COM

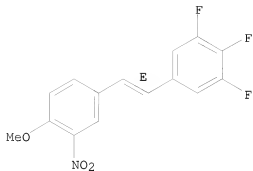
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3-trifluoro-5-[(1E)-2-(4-methoxy-3-nitrophenyl)ethenyl]-  
 MF C15 H10 F3 N O3

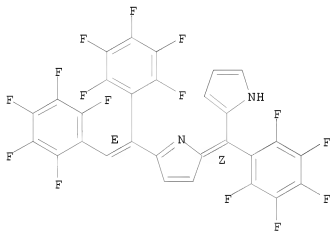
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

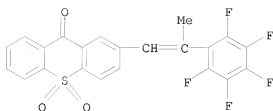
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 1H-Pyrrole, 2-[(2)-[5-(1E)-1,2-bis(2,3,4,5,6-pentafluorophenyl)ethenyl]-  
2H-pyrrol-2-ylidene](2,3,4,5,6-pentafluorophenyl)methyl]-  
MF C29 H7 F15 N2

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

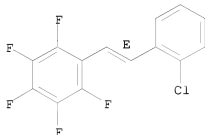
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 9H-Thioxanthen-9-one, 2-[2-(2,3,4,5,6-pentafluorophenyl)-1-propen-1-yl]-,  
10,10-dioxide  
MF C22 H11 F5 O3 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, [(1E)-2-(2-chlorophenyl)ethenyl]pentafluoro- (9CI)  
 MF C14 H6 Cl F5

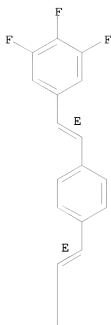
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Bicyclo[2.2.2]octane, 1-propyl-4-[(1E)-2-[4-[(1E)-2-(3,4,5-trifluorophenyl)ethenyl]phenyl]ethenyl]-  
 MF C27 H29 F3

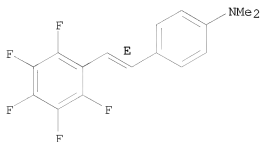
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

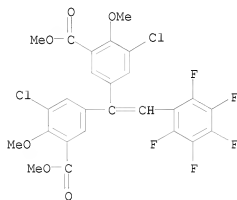
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenamine, N,N-dimethyl-4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-  
 MF C16 H12 F5 N

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

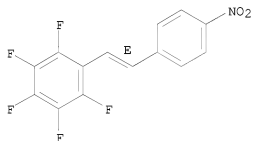
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzoic acid, 3,3'-[(pentafluorophenyl)ethenylidene]bis[5-chloro-6-methoxy-  
dimethyl ester (9CI)  
MF C26 H17 Cl2 F5 O6



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, pentafluoro[(1E)-2-(4-nitrophenyl)ethenyl]- (9CI)  
MF C14 H6 F5 N O2

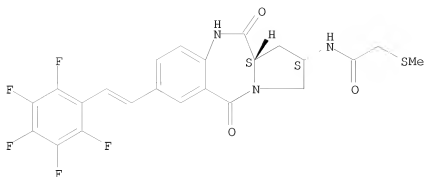
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

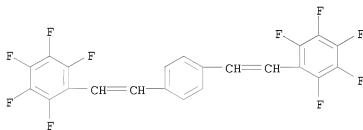
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Acetamide, N-[(2S,11aS)-2,3,5,10,11,11a-hexahydro-5,11-dioxo-7-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-1H-pyrrolo[2,1-c][1,4]benzodiazepin-2-yl]-2-(methylthio)-  
MF C23 H18 F5 N3 O3 S

Absolute stereochemistry.  
Double bond geometry unknown.



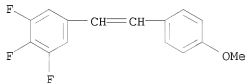
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,4-bis[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-  
 MF C22 H8 F10



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

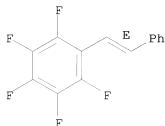
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3-trifluoro-5-[2-(4-methoxyphenyl)ethenyl]-  
 MF C15 H11 F3 O



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-phenylethenyl]-  
 MF C14 H7 F5

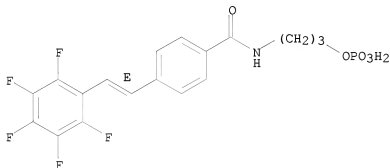
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzamide, 4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-N-[3-(  
(phosphonooxy)propyl)-  
MF C18 H15 F5 N O5 P

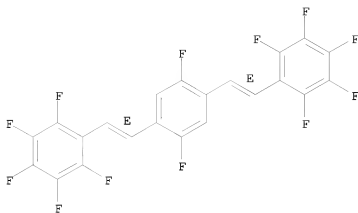
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, 1,4-difluoro-2,5-bis[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-  
MF C22 H6 F12

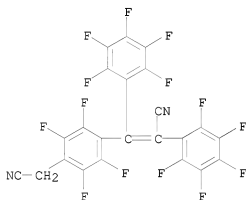
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile,  $\alpha$ -[4-(cyanomethyl)-2,3,5,6-tetrafluorophenyl](2,3,4,5,6-pentafluorophenyl)methylene]-2,3,4,5,6-pentafluoro-, compd. with 1-butanamine (1:1)  
 MF C23 H2 F14 N2 . C4 H11 N

CM 1



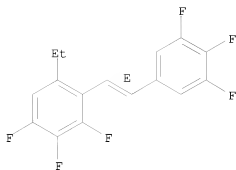
CM 2



L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1-ethyl-3,4,5-trifluoro-2-[(1E)-2-(3,4,5-trifluorophenyl)ethenyl]-  
 MF C16 H10 F6

Double bond geometry as shown.

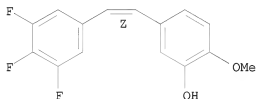




\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Phenol, 2-methoxy-5-[(1Z)-2-(3,4,5-trifluorophenyl)ethenyl]-  
 MF C15 H11 F3 O2

Double bond geometry as shown.

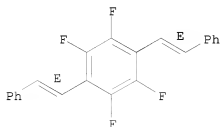


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,4,5-tetrafluoro-3,6-bis(2-phenylethenyl)-, stereoisomer,  
 compd. with (E,E)-1,4-bis[2-(pentafluorophenyl)ethenyl]benzene (1:1) (9CI)  
 MF C22 H14 F4 . C22 H8 F10

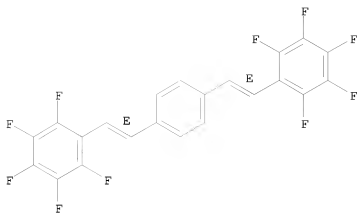
CM 1

Double bond geometry as shown.

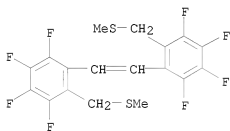


CM 2

Double bond geometry as shown.



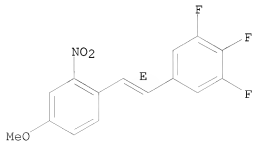
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-(1,2-ethenediyl)bis[2,3,4,5-tetrafluoro-6-  
 [(methylthio)methyl]-  
 MF C18 H12 F8 S2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3-trifluoro-5-[(1E)-2-(4-methoxy-2-nitrophenyl)ethenyl]-  
 MF C15 H10 F3 N O3

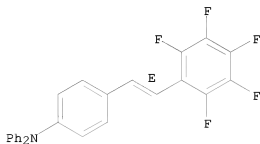
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzenamine, 4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-N,N-diphenyl-  
MF C26 H16 F5 N

Double bond geometry as shown.

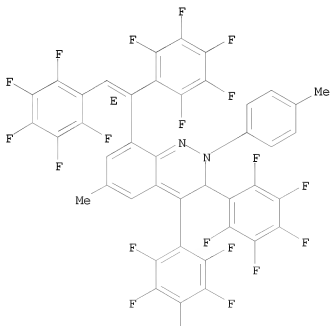


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Cinnoline, 8-[1,2-bis(pentafluorophenyl)ethenyl]-2,3-dihydro-6-methyl-2-(4-methylphenyl)-3,4-bis(pentafluorophenyl)-, (E)- (9CI)  
MF C42 H14 F20 N2

Double bond geometry as shown.

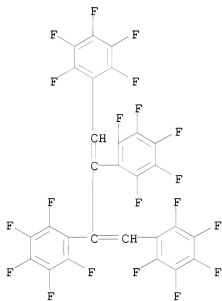
PAGE 1-A





\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1',1'',1'''-(1,3-butadiene-1,2,3,4-tetrayl)tetrakis[2,3,4,5,6-  
 pentafluoro-  
 MF C28 H2 F20

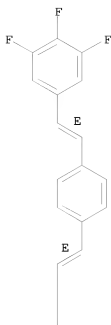


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Bicyclo[2.2.2]octan-1-ol, 4-[(1E)-2-[4-[(1E)-2-(3,4,5-  
 trifluorophenyl)ethenyl]phenyl]ethenyl]-  
 MF C24 H23 F3 O

Double bond geometry as shown.

PAGE 1-A



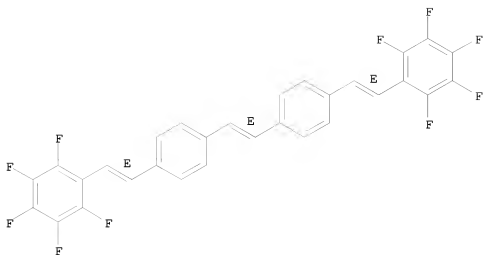
PAGE 2-A



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

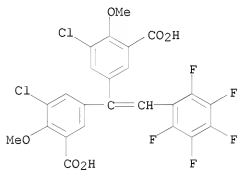
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, 1,1'-(1E)-1,2-ethenediylbis[4-[(1E)-2-(pentafluorophenyl)ethenyl]-  
(9CI)  
MF C30 H14 F10

Double bond geometry as shown.



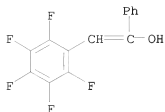
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzoic acid, 3,3'-[(pentafluorophenyl)ethenylidene]bis[5-chloro-6-methoxy-  
 , diammonium salt (9CI)  
 MF C24 H13 Cl2 F5 O6 . 2 H3 N



● 2 NH<sub>3</sub>

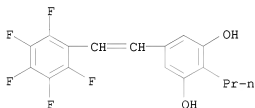
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenemethanol, α-[(2,3,4,5,6-pentafluorophenyl)methylene]-, sodium  
 salt (1:1)  
 MF C14 H7 F5 O . Na



● Na

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

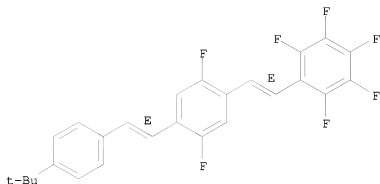
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 1,3-Benzenediol, 5-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-2-propyl-  
 MF C17 H13 F5 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

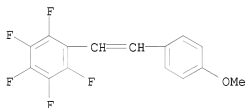
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1-[(1E)-2-[4-(1,1-dimethylethyl)phenyl]ethenyl]-2,5-difluoro-4-  
 [(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-  
 MF C26 H19 F7

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3,4,5-pentafluoro-6-[2-(4-methoxyphenyl)ethenyl]-  
 MF C15 H9 F5 O

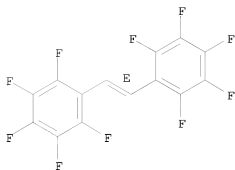


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-(1E)-1,2-ethenediylbis[2,3,4,5,6-pentafluoro-  
 MF C14 H2 F10  
 CI COM

Double bond geometry as shown.

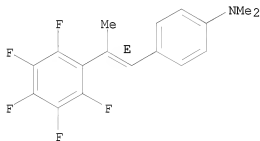




\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

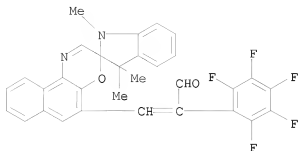
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenamine, N,N-dimethyl-4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)-1-propen-  
 1-yl]-  
 MF C17 H14 F5 N

Double bond geometry as shown.



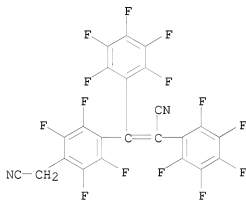
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetaldehyde,  $\alpha$ -[(1,3-dihydro-1,3,3-trimethylspiro[2H-indole-  
 2,3'-[3H]naphth[2,1-b][1,4]oxazin]-5'-yl)methylene]-2,3,4,5,6-pentafluoro-  
 MF C31 H21 F5 N2 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

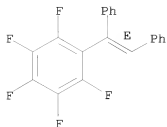
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile,  $\alpha$ -[4-(cyanomethyl)-2,3,5,6-tetrafluorophenyl](2,3,4,5,6-pentafluorophenyl)methylene]-2,3,4,5,6-pentafluoro-  
 MF C23 H2 F14 N2  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1-[(1E)-1,2-diphenylethenyl]-2,3,4,5,6-pentafluoro-  
 MF C20 H11 F5

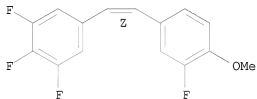
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3-trifluoro-5-[(1Z)-2-(3-fluoro-4-methoxyphenyl)ethenyl]-  
 MF C15 H10 F4 O

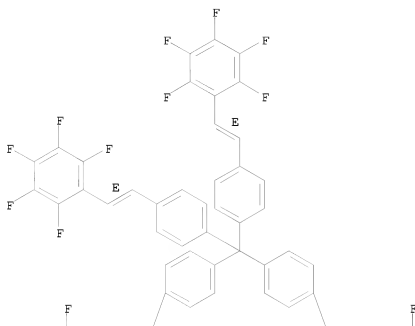
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1',1'',1'''-methanetetrayltetrakis[4-[2-(  
 pentafluorophenyl)ethenyl]-, (all-E)- (9CI)  
 MF C57 H24 F20

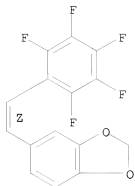
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 1,3-Benzodioxole, 5-[2-(pentafluorophenyl)ethynyl]-, (Z)- (9CI)  
 MF C15 H7 F5 O2

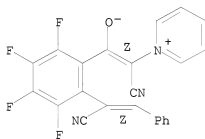
Double bond geometry as shown.



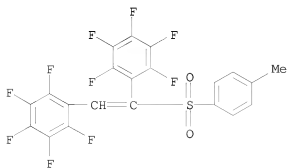
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Pyridinium, 1-[(1Z)-1-cyano-2-[2-[(1Z)-1-cyano-2-phenylethenyl]-3,4,5,6-tetrafluorophenyl]-2-hydroxyethenyl]-, inner salt  
 MF C23 H11 F4 N3 O

Double bond geometry as shown.

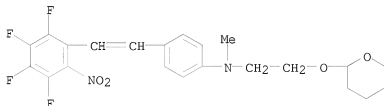


L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-[1-[(4-methylphenyl)sulfonyl]-1,2-ethenediyl]bis[2,3,4,5,6-pentafluoro- (9CI)  
 MF C21 H8 F10 O2 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

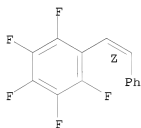
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzenamine, N-methyl-4-[2-(2,3,4,5-tetrafluoro-6-nitrophenyl)ethenyl]-N-  
MF [2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl]-  
C22 H22 F4 N2 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, 1,2,3,4,5-pentafluoro-6-[(1Z)-2-phenylethenyl]-  
MF C14 H7 F5

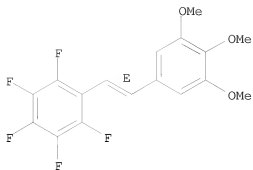
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-(3,4,5-trimethoxyphenyl)ethenyl]-  
MF C17 H13 F5 O3

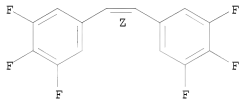
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-(1Z)-1,2-ethenediylbis[3,4,5-trifluoro- (9CI)  
 MF C14 H6 F6

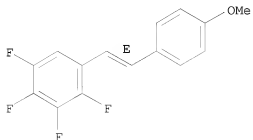
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3,4-tetrafluoro-5-[2-(4-methoxyphenyl)ethenyl]-, (E)- (9CI)  
 MF C15 H10 F4 O

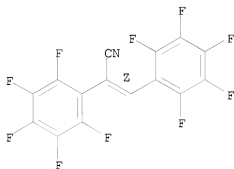
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Acrylonitrile, 2,3-bis(pentafluorophenyl)-, (Z)- (8CI)  
 MF C15 H F10 N

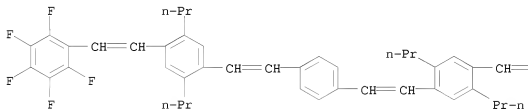
Double bond geometry as shown.



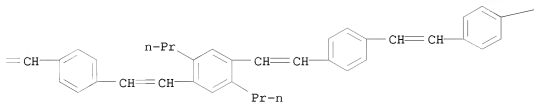
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1-[2-[4-[2-[4-[2-[4-(4-methoxyphenyl)ethenyl]phenyl]ethenyl]-  
 2,5-dipropylphenyl]ethenyl]phenyl]ethenyl]-4-[2-[4-[2-[4-[2-(2,3,4,5,6-  
 pentafluorophenyl)ethenyl]-2,5-dipropylphenyl]ethenyl]phenyl]ethenyl]-2,5-  
 dipropyl-  
 MF C81 H81 F5 O

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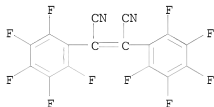
PAGE 1-C

— OMe



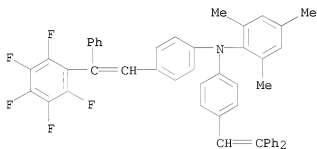
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 2-Butenedinitrile, 2,3-bis(pentafluorophenyl)-, radical ion(1-),  
 vanadium(2+), (2E)- (9CI)  
 MF C16 F10 N2 . 1/2 V  
 CI COM, RIS



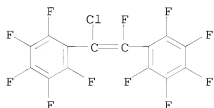
● 1/2 V(II) 2+

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenamine, N-[4-(2,2-diphenylethenyl)phenyl]-2,4,6-trimethyl-N-[4-(2-  
 (2,3,4,5,6-pentafluorophenyl)-2-phenylethenyl)phenyl]-  
 MF C49 H36 F5 N



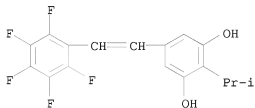
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Stilbene,  $\alpha$ -chloroundecafluoro- (7CI, 8CI)  
 MF C14 Cl F11



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 1,3-Benzenediol, 2-(1-methylethyl)-5-[2-(2,3,4,5,6-  
 pentafluorophenyl)ethenyl]-  
 MF C17 H13 F5 O2

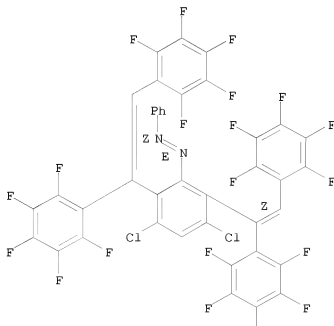


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Diazene, 1-[2,6-bis[(1Z)-1,2-bis(2,3,4,5,6-pentafluorophenyl)ethenyl]-3,5-  
 dichlorophenyl]-2-phenyl-, (1E)-  
 MF C40 H8 Cl2 F20 N2

Double bond geometry as shown.

PAGE 1-A

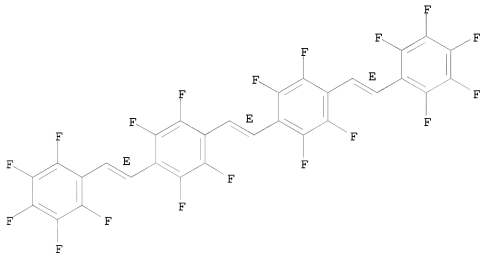


F

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

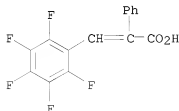
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-(1,2-ethenediyl)bis[2,3,5,6-tetrafluoro-4-[2-(  
 pentafluorophenyl)ethenyl]-, (E,E,E)- (9CI)  
 MF C30 H6 F18

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

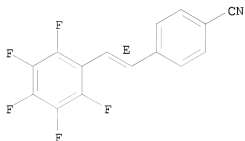
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenecarboxylic acid, α-[(2,3,4,5,6-pentafluorophenyl)methylene]-  
 MF C15 H7 F5 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzonitrile, 4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-  
 MF C15 H6 F5 N

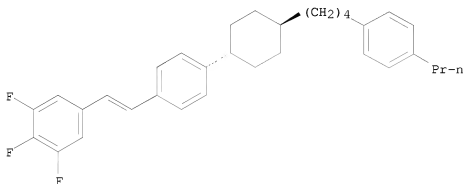
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1-[trans-4-[4-(4-propylphenyl)butyl]cyclohexyl]-4-[2-(3,4,5-trifluorophenyl)ethenyl]-  
 MF C33 H37 F3

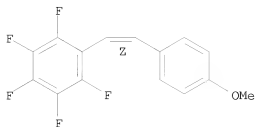
Relative stereochemistry.  
 Double bond geometry unknown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, pentafluoro[2-(4-methoxyphenyl)ethenyl]-, (Z)- (9CI)  
 MF C15 H9 F5 O

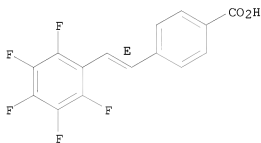
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

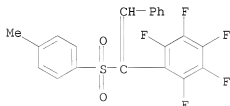
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzoic acid, 4-[(1E)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-  
 MF C15 H7 F5 O2

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

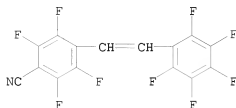
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3,4,5-pentafluoro-6-[1-[(4-methylphenyl)sulfonyl]-2-  
 phenylethenyl]-  
 MF C21 H13 F5 O2 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

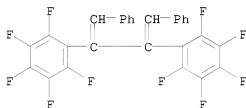
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzonitrile, 2,3,5,6-tetrafluoro-4-[2-(2,3,4,5,6-

MF pentafluorophenyl)ethenyl)-  
C15 H2 F9 N



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

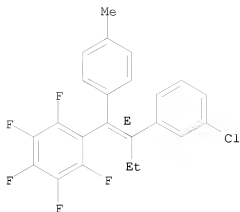
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, 1,1'-[1,2-bis(phenylmethylene)-1,2-ethanediyl]bis[2,3,4,5,6-  
pentafluoro- (9CI)  
MF C28 H12 F10



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, 1-[(1E)-2-(3-chlorophenyl)-1-(4-methylphenyl)-1-buten-1-yl]-  
2,3,4,5,6-pentafluoro-  
MF C23 H16 Cl F5

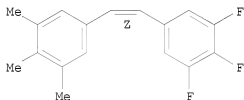
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3-trifluoro-5-[(1Z)-2-(3,4,5-trimethylphenyl)ethenyl]-  
 MF C17 H15 F3

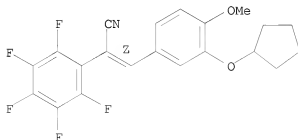
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

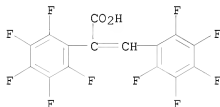
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile,  $\alpha$ -[[3-(cyclopentyloxy)-4-methoxyphenyl]methylene]-2,3,4,5,6-pentafluoro-, (Z)- (9CI)  
 MF C21 H16 F5 N O2

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

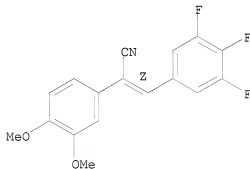
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzeacetic acid, 2,3,4,5,6-pentafluoro- $\alpha$ -(2,3,4,5,6-pentafluorophenyl)methylene)-  
MF C15 H2 F10 O2  
CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzeacetonitrile, 3,4-dimethoxy- $\alpha$ -(3,4,5-trifluorophenyl)methylene)-, ( $\alpha$ Z)-  
MF C17 H12 F3 N O2

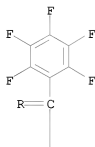
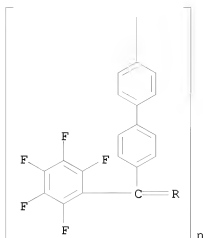
Double bond geometry as shown.



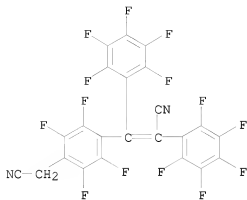
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Poly[[1,1'-biphenyl]-4,4'-diyl{(1E)-1,2-bis(pentafluorophenyl)-1,2-ethenediyl}] (9CI)  
MF (C26 H8 F10)n  
CI PMS





L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile,  $\alpha$ -[[4-(cyanomethyl)-2,3,5,6-  
 tetrafluorophenyl](2,3,4,5,6-pentafluorophenyl)methylene]-2,3,4,5,6-  
 pentafluoro-, compd. with N-butyl-1-butanamine (1:1)  
 MF C23 H2 F14 N2 . C8 H19 N

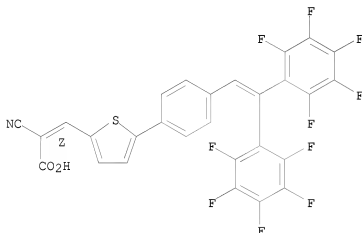


CM 2

n-Bu-NH-Bu-n

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 2-Propenoic acid, 3-[5-[4-[2,2-bis(2,3,4,5,6-pentafluorophenyl)ethenyl]phenyl]-2-thienyl]-2-cyano-, (2Z)-  
 MF C28 H9 F10 N O2 S

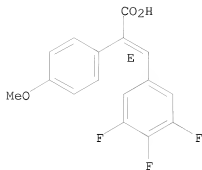
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetic acid, 4-methoxy- $\alpha$ -[(3,4,5-trifluorophenyl)methylene]-,  
 ( $\alpha$ E)-  
 MF C16 H11 F3 O3

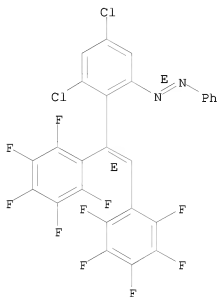
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

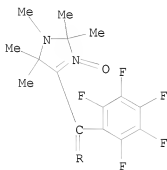
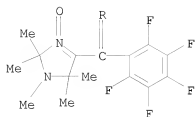
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Diazene, 1-[2-[(1E)-1,2-bis(2,3,4,5,6-pentafluorophenyl)ethenyl]-3,5-  
 dichlorophenyl]-2-phenyl-, (1E)-  
 MF C26 H8 Cl2 F10 N2

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

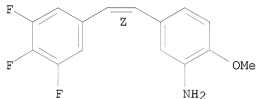
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 1H-imidazole, 4,4'-[1,2-bis(pentafluorophenyl)-1,2-ethenediyl]bis[2,5-  
 dihydro-1,2,2,5,5-pentamethyl-, 3,3'-dioxide (9CI)  
 MF C30 H30 F10 N4 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenamine, 2-methoxy-5-[(1Z)-2-(3,4,5-trifluorophenyl)ethenyl]-  
 MF C15 H12 F3 N O

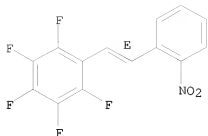
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

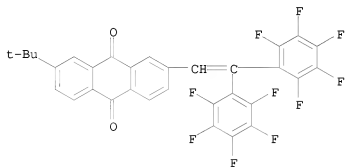
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-(2-nitrophenyl)ethenyl]-  
 MF C14 H6 F5 N O2

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

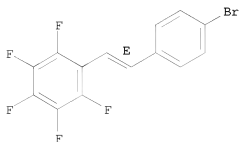
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 9,10-Anthracenedione, 2-[2,2-bis(2,3,4,5,6-pentafluorophenyl)ethenyl]-7-(  
 (1,1-dimethylethyl)-  
 MF C32 H16 F10 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1-[(1E)-2-(4-bromophenyl)ethenyl]-2,3,4,5,6-pentafluoro-  
 MF C14 H6 Br F5

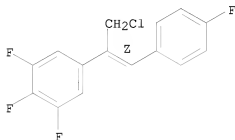
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, 5-[(1Z)-1-(chloromethyl)-2-(4-fluorophenyl)ethenyl]-1,2,3-  
trifluoro-  
MF C15 H9 Cl F4

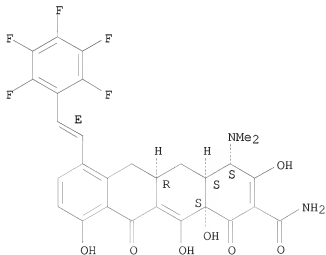
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-  
3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[(1E)-2-(2,3,4,5,6-  
pentafluorophenyl)ethenyl]-, (4S,4aS,5aR,12aS)-  
MF C29 H23 F5 N2 O7

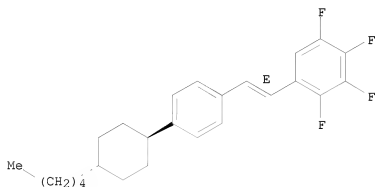
Absolute stereochemistry.  
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

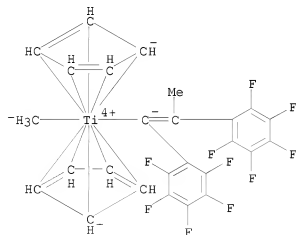
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3,4-tetrafluoro-5-[2-[4-(4-pentylcyclohexyl)phenyl]ethenyl]-,  
 [1 $\alpha$ (E),4 $\beta$ ]- (9CI)  
 MF C25 H28 F4

Relative stereochemistry.  
 Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

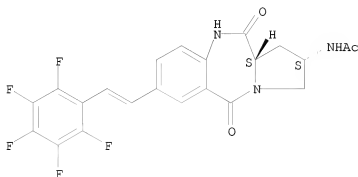
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Titanium, [1,2-bis(pentafluorophenyl)-1-propenyl]bis( $\eta$ 5-2,4-cyclopentadien-1-yl)methyl- (9CI)  
 MF C26 H16 F10 Ti  
 CI CCS



L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Acetamide, N-[(2S,11aS)-2,3,5,10,11,11a-hexahydro-5,11-dioxo-7-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-1H-pyrrolo[2,1-c][1,4]benzodiazepin-

2-yl]-  
MF C22 H16 F5 N3 O3

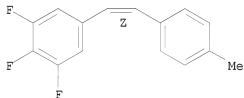
Absolute stereochemistry.  
Double bond geometry unknown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, 1,2,3-trifluoro-5-[(1Z)-2-(4-methylphenyl)ethenyl]-  
MF C15 H11 F3

Double bond geometry as shown.

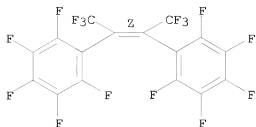


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, 1,1'-[1,2-bis(trifluoromethyl)-1,2-ethenediyl]bis[2,3,4,5,6-  
pentafluoro-, (Z)- (9CI)  
MF C16 F16

Double bond geometry as shown.



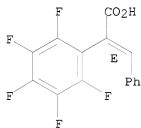


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

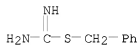
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Acrylic acid, 2-(pentafluorophenyl)-3-phenyl-, compd. with  
 2-benzyl-2-thiopseudourea (1:1), (E)- (8CI)  
 MF C15 H7 F5 O2 . C8 H10 N2 S

CM 1

Double bond geometry as shown.

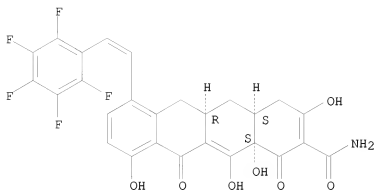


CM 2



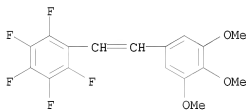
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 2-Naphthacenecarboxamide, 1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-  
 tetrahydroxy-1,11-dioxo-7-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-,  
 (4aS,5aR,12aS)-  
 MF C27 H18 F5 N O7

Absolute stereochemistry.  
 Double bond geometry unknown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

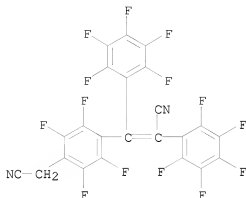
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3,4,5-pentafluoro-6-[2-(3,4,5-trimethoxyphenyl)ethenyl]-  
 MF C17 H13 F5 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile,  $\alpha$ -[4-(cyanomethyl)-2,3,5,6-tetrafluorophenyl](2,3,4,5,6-pentafluorophenyl)methylene]-2,3,4,5,6-pentafluoro-, compd. with N-propyl-1-propanamine (1:1)  
 MF C23 H2 F14 N2 . C6 H15 N

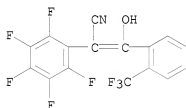
CM 1



CM 2

n-Pr-NH-Pr-n

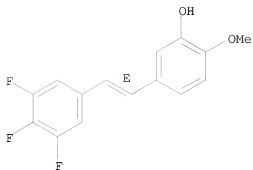
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile, 2,3,4,5,6-pentafluoro- $\alpha$ -[hydroxy[2-(trifluoromethyl)phenyl]methylene]-  
 MF C16 H5 F8 N O



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

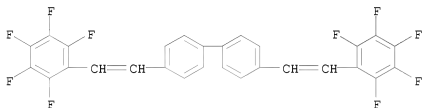
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Phenol, 2-methoxy-5-[(1E)-2-(3,4,5-trifluorophenyl)ethenyl]-  
 MF C15 H11 F3 O2

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

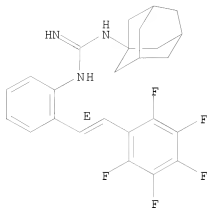
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 1,1'-Biphenyl, 4,4'-bis[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-  
 MF C28 H12 F10



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Guanidine, N-[2-[2-(pentafluorophenyl)ethenyl]phenyl]-N'-  
 tricyclo[3.3.1.1.3,7]dec-1-yl-, (E)- (9CI)  
 MF C25 H24 F5 N3  
 CI COM

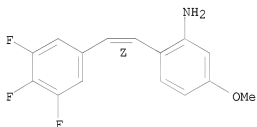
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenamine, 5-methoxy-2-[(1Z)-2-(3,4,5-trifluorophenyl)ethenyl]-  
 MF C15 H12 F3 N O

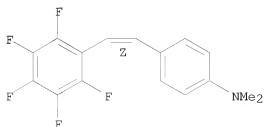
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

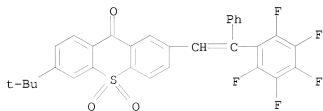
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenamine, N,N-dimethyl-4-[(1Z)-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-  
 MF C16 H12 F5 N

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

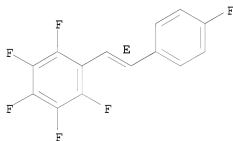
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 9H-Thioxanthen-9-one, 6-(1,1-dimethylethyl)-2-[2-(2,3,4,5,6-pentafluorophenyl)-2-phenylethenyl]-, 10,10-dioxide  
MF C31 H21 F5 O3 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, pentafluoro[2-(4-fluorophenyl)ethenyl]-, (E)- (9CI)  
MF C14 H6 F6

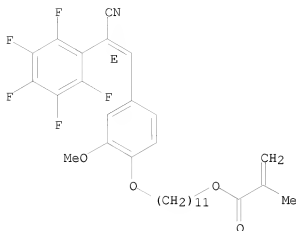
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

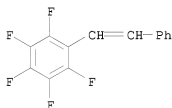
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN 2-Propenoic acid, 2-methyl-, 11-[4-[(1E)-2-cyano-2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-2-methoxyphenoxy]undecyl ester  
MF C31 H34 F5 N O4

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

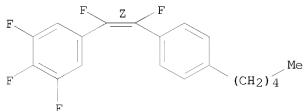
L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,2,3,4,5-pentafluoro-6-(2-phenylethenyl)-  
 MF C14 H7 F5  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 5-[1,2-difluoro-2-(4-pentylphenyl)ethenyl]-1,2,3-trifluoro-, (Z)-  
 (9CI)  
 MF C19 H17 F5

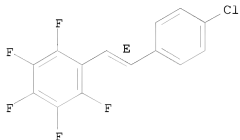
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, [(1E)-2-(4-chlorophenyl)ethenyl]pentafluoro- (9CI)  
MF C14 H6 Cl F5

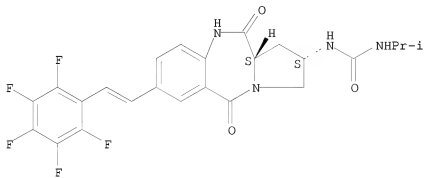
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Urea, N-[(2S,11aS)-2,3,5,10,11,11a-hexahydro-5,11-dioxo-7-[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-1H-pyrrolo[2,1-c][1,4]benzodiazepin-2-yl]-N'-(1-methylethyl)-  
MF C24 H21 F5 N4 O3

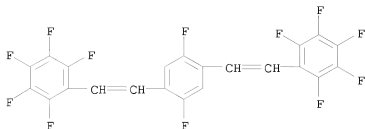
Absolute stereochemistry.  
Double bond geometry unknown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
IN Benzene, 1,4-difluoro-2,5-bis[2-(2,3,4,5,6-pentafluorophenyl)ethenyl]-  
MF C22 H6 F12

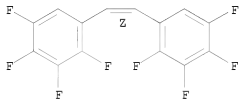




\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzene, 1,1'-(1,2-ethenediyl)bis[2,3,4,5-tetrafluoro-, (Z)- (9CI)  
 MF C14 H4 F8

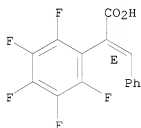
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 201 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Acrylic acid, 2-(pentafluorophenyl)-3-phenyl-, (E)- (8CI)  
 MF C15 H7 F5 O2  
 CI COM

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> fil capl  
 COST IN U.S. DOLLARS

SINCE FILE TOTAL

FULL ESTIMATED COST

ENTRY	SESSION
194.04	194.48

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USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

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=> s l4

L5 152 L4

=> d ibib abs hitstr 150-152

L5 ANSWER 150 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1967:500075 CAPLUS  
DOCUMENT NUMBER: 67:100075  
ORIGINAL REFERENCE NO.: 67:18823a,18826a  
TITLE: Reaction of pentafluorobenzonitrile with hydroxylamine  
AUTHOR(S): Shchegoleva, G. S.; Barkhash, V. A.; Vorozhtsov, N. N., Jr.  
CORPORATE SOURCE: Novosibirsk Inst. Organ. Khim., Novosibirsk, USSR  
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1967), (3), 708-9  
CODEN: IASKA6; ISSN: 0002-3353  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
GI For diagram(s), see printed CA Issue.  
AB cf. CA 64: 12586d. To 1 g. C6F5CN and 1.4 g. HONH2.HCl in EtOH at 0° was added slowly 0.8 g. Na2CO3 in H2O, the mixture kept 6 hrs. at 0°, extracted with Et2O, and the evaporated extract treated with 24% HBr gave

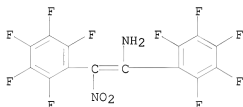
64% 2,3,4,5,6-pentafluorobenzamidoxime-HBr, m. 193-6°; free oxime (I) m. 94-7° (after sublimation). I (0.5 g.) and 1.5 g. C6F5COCl heated 0.5 hr. in C6H6 gave 80% C6F5C(NH2):NO2CC6F5 (II), m. 147-51°. BzCl similarly gave the benzoate, m. 160-5°. Refluxing II with POCl3 3 hrs. gave, after treatment with ice, 96% 3,5-bis(pentafluorophenyl)-1,2,4-oxadiazole (III), m. 100-1°. Similarly was prepared 3-pentafluorophenyl-5-phenyl-1,2,4-oxadiazole (IV), m. 88-93°. Ir spectra are reported, along with N.M.R. spectra, which confirmed the above structures.

IT 1081539-80-1P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)  
(Reaction of pentafluorobenzonitrile with hydroxylamine)

RN 1081539-80-1 CAPLUS

CN Benzenemethanamine, 2,3,4,5,6-pentafluoro- $\alpha$ -[nitro(2,3,4,5,6-pentafluorophenyl)methylene]- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
(1 CITINGS)

L5 ANSWER 151 OF 152 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 1967:421520 CAPLUS

DOCUMENT NUMBER: 67:21520

ORIGINAL REFERENCE NO.: 67:4055a,4058a

TITLE: Polyfluoroarenes. IX. Decafluorotolan: synthesis, properties, and use as an organometallic ligand  
BIRCHALL, John M.; BOWDEN, F. L.; HASZELDINE, Robert N.; LEVER, Alfred B. P.

CORPORATE SOURCE: Univ. Manchester, Manchester, UK

SOURCE: Journal of the Chemical Society [Section] A: Inorganic, Physical, Theoretical (1967), (5), 747-53  
CODEN: JCSIAP; ISSN: 0022-4944

DOCUMENT TYPE: Journal

LANGUAGE: English

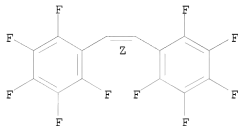
AB cf. CA 66: 37126j. IC.tplbond.CI and C6F5MgBr give decafluorotolan (C6F5C.tplbond.CC6F5) in good yield. The triple bond in the tolan undergoes ready catalytic hydrogenation, addition of Br, and oxidative cleavage, but is relatively unreactive towards hydration, iodination, and carbonylation. Decafluorotolan reacts with methoxide ion in the 4- and 4'-positions, and gives a good yield of tetrakis(pentafluorophenyl)thiophene when it is heated with S. Reaction of the tolan with Co octacarbonyl yields a complex Co2(CO)6(C6F5C.tplbond.CC6F5), shown by its chemical and spectroscopic properties to be similar in structure to its hydrocarbon analog; octafluoro-4,4'-dimethoxytolan behaves similarly. Tetrakis(pentafluorophenyl)cyclopentadienone (perfluorotetracyclone) is obtained when a solution of the Co carbonyl complex of decafluorotolan is heated. Reaction of decafluorotolan with Fe penta- or dodecacarbonyl yields a complex Fe2(CO)6(C6F5C.tplbond.CC6F5)2, together with perfluorotetracyclone. 21 references.

IT 14992-38-2P 14992-40-6P 14992-41-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

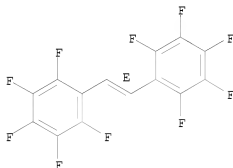
(preparation of)  
 RN 14992-38-2 CAPLUS  
 CN Benzene, 1,1'-(1Z)-1,2-ethenediylbis[2,3,4,5,6-pentafluoro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

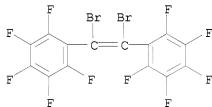


RN 14992-40-6 CAPLUS  
 CN Benzene, 1,1'-(1E)-1,2-ethenediylbis[2,3,4,5,6-pentafluoro- (CA INDEX NAME)

Double bond geometry as shown.



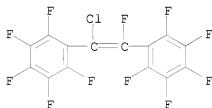
RN 14992-41-7 CAPLUS  
 CN Benzene, 1,1'-(1,2-dibromo-1,2-ethenediyl)bis[2,3,4,5,6-pentafluoro- (CA INDEX NAME)



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD  
 (6 CITINGS)

L5 ANSWER 152 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1966:67439 CAPLUS  
 DOCUMENT NUMBER: 64:67439  
 ORIGINAL REFERENCE NO.: 64:12576a-c  
 TITLE: Aromatic polyfluoro compounds. XXVIII. Further reactions of the pentafluorophenyl anion

AUTHOR(S): Callander, D. D.; Coe, P. L.; Tatlow, J. C.  
 CORPORATE SOURCE: Univ. Birmingham, UK  
 SOURCE: Tetrahedron (1966), 22(2), 419-32  
 CODEN: TETRAB; ISSN: 0040-4020  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB cf. CA 64, 1987f. The pentafluorophenyl anion from pentafluorophenyllithium was used as a nucleophile and as a source of tetrafluorobenzene. As a nucleophile, it was used to make polyfluorobenzene and -terphenyl derivs. from perfluorotoluene, perfluoro-o-xylene, pentafluoronitrobenzene and bromopentafluorobenzene, and polyfluoropolyaryls from perfluorobiphenyl. It also attacked decafluorocyclohexene and chlorotrifluoroethylene, presumably by an addition-elimination sequence. Reactions using the tetrafluorobenzene intermediate were carried out in the presence of excess bromopentafluorobenzene, pentafluorobenzene, and various lithium halides, in some cases with variation of the solvent. A mechanism for some of these reactions is postulated.  
 IT 5576-21-6P, Stilbene,  $\alpha$ -chloroundecafluoro-  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 5576-21-6 CAPLUS  
 CN Stilbene,  $\alpha$ -chloroundecafluoro- (7CI, 8CI) (CA INDEX NAME)



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD  
 (7 CITINGS)

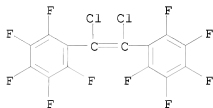
=> d ibib abs hitstr 140-149

L5 ANSWER 140 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1973:546162 CAPLUS  
 DOCUMENT NUMBER: 79:146162  
 ORIGINAL REFERENCE NO.: 79:23689a,23692a  
 TITLE: Decafluoro- $\alpha,\beta$ -dichlorostilbene  
 INVENTOR(S): Dvornikova, K. V.; Platonov, V. E.; Jakobson, G. G.  
 PATENT ASSIGNEE(S): Novosibirsk Institute of Organic Chemistry  
 SOURCE: U.S.S.R. From: Otkrytiya, Izobret., Prom. Obraztsy,  
 Tovarnye Znaki 1973, 50(32), 49.  
 CODEN: URXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Russian  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 392060	A1	19730727	SU 1971-1690000	19710804
PRIORITY APPLN. INFO.:			SU 1971-1690000	A 19710804

AB (C6F5CCl)<sub>2</sub> was prepared by heating C6F5CCl<sub>3</sub> in the presence of Cu at 400-500° or at 150-200° in a closed system.

IT 49763-76-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 49763-76-0 CAPLUS  
 CN Benzene, 1,1'-(1,2-dichloro-1,2-ethenediyl)bis[2,3,4,5,6-pentafluoro- (CA  
 INDEX NAME)



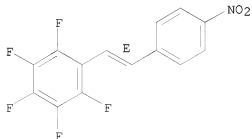
L5 ANSWER 141 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1972:501784 CAPLUS  
 DOCUMENT NUMBER: 77:101784  
 ORIGINAL REFERENCE NO.: 77:16783a,16786a  
 TITLE: Reaction of phosphorus ylides with perfluorobenzene  
 AUTHOR(S): Nesmeyanov, N. A.; Berman, S. T.; Reutov, O. A.  
 CORPORATE SOURCE: Mosk. Gos. Univ. im. Lomonosova, Moscow, USSR  
 SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya  
 (1972), (3), 605-6  
 CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE: Journal  
 LANGUAGE: Russian

AB Under argon, MePh3PI and PhLi in Et2O-C6H6, kept 2.5 hr, filtered and treated with C6F6 2 hr, gave Ph3P:C(C6F5)H which was treated in situ with p-O2NC6H4CHO 12 hr to give 62% trans-C6F5CH:CHC6-H4NO2-p. Similarly formed was the p-Cl analog (51%). Ph2P(CH2Ph)Cl treated with BuLi in THF-Et2O gave the corresponding ylide in solution, which was treated with C6F6 to give a solution of Ph3P+CH(C6F5)Ph F- (I). I reacted with the residual ylide to form Ph3P:CPhC6F5 (II) in solution along with Ph3P+CH2Ph F-. Treated with aqueous NH4BF4, this gave PhCH2P+Ph3-BF4 while the organic phase gave 85% II. II with dry HCl formed the conjugate acid, which reverted to the ylide on contact with a nucleophile, e.g., aqueous Na2CO3.

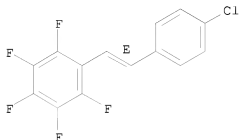
IT 37516-14-6P 37516-15-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 37516-14-6 CAPLUS  
 CN Benzene, pentafluoro[(1E)-2-(4-nitrophenyl)ethenyl]- (9CI) (CA INDEX  
 NAME)

Double bond geometry as shown.



RN 37516-15-7 CAPLUS  
 CN Benzene, [(1E)-2-(4-chlorophenyl)ethenyl]pentafluoro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L5 ANSWER 142 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1971:469273 CAPLUS

DOCUMENT NUMBER: 75:69273

ORIGINAL REFERENCE NO.: 75:10951a,10954a

TITLE: Aromatic fluorinated derivatives. XLIII. Equilibrium acidity of pentafluorophenyl methanes

AUTHOR(S): Vlasov, V. M.; Krivousova, E. D.; Yakobson, G. G.

CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1971), 7(5), 986-9

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal

LANGUAGE: Russian

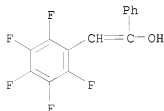
AB The reaction of NaH with C6F5CH2COPh (I) in MeOCH2CH2OMe solution gives C6F5CH:CPHO-Na+ (II). Similarly, C6F5CH:C(C6F5)O-Na+ (III) is obtained. NMR spectra of p- and m- F atoms of II and III show more pos. chemical shifts than the spectra of I or C6F5CH2COC6F5 (IV). PK values of I and IV are resp. 15.3 and 11.7. This pK shift, which is due to the replacement of Ph with C6F5, is considerably greater than expected because of the relatively small contribution of resonance towards the stabilization of II or III carbanions.

IT 33753-91-2 33753-92-3

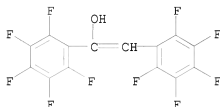
RL: PRP (Properties)  
 (nuclear magnetic resonance of)

RN 33753-91-2 CAPLUS

CN Benzenemethanol,  $\alpha$ -(2,3,4,5,6-pentafluorophenyl)methylene]-, sodium salt (1:1) (CA INDEX NAME)



RN 33753-92-3 CAPLUS  
 CN Benzenemethanol, 2,3,4,5,6-pentafluoro- $\alpha$ -(2,3,4,5,6-pentafluorophenyl)methylene]-, sodium salt (1:1) (CA INDEX NAME)

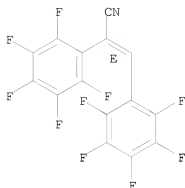


● Na

L5 ANSWER 143 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1970:31402 CAPLUS  
 DOCUMENT NUMBER: 72:31402  
 ORIGINAL REFERENCE NO.: 72:5717a,5720a  
 TITLE: Aromatic fluoro-derivatives. XXXVII. Reaction of pentafluorophenylacetonitrile with aldehydes in the presence of potassium fluoride  
 AUTHOR(S): Vlasov, V. M.; Yakobson, G. G.  
 CORPORATE SOURCE: Novosibirsk. Inst. Org. Khim., Novosibirsk, USSR  
 SOURCE: Zhurnal Obshchei Khimii (1969), 39(9), 2071-5  
 CODEN: ZOKHA4; ISSN: 0044-460X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 AB C6F5CH2CN (I) and paraformaldehyde kept 7 hr in (CH2OMe)2 in the presence of KF gave 42% C6F5CH(CN)CH2OH ("pentafluoroacetonitrile"), b0.2 110-12°, m. 41.5-2.5°, and 22% CH2[CH(CN)C6F5]2, m. 100-11°, both characterized by NMR and ir spectra. Similar reaction but with C6F5CHO in the presence of KF converted I into 17% cis-decafluorocyanostilbene, m. 103-5°, its mixture with the trans isomer (2%), m. 85-95°; and 8% 1,2-bis(pentafluorophenyl)-2-cyanoethanol, m. 146-8.5°; all were characterized by NMR spectra; the residue gave some C6F5CH2CONH2, m. 178-81.5°. Thus KF catalyzes condensations of I with aldehydes.  
 IT 25529-43-5P 25576-30-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 25529-43-5 CAPLUS  
 CN Acrylonitrile, 2,3-bis(pentafluorophenyl)-, (E)- (8CI) (CA INDEX NAME)

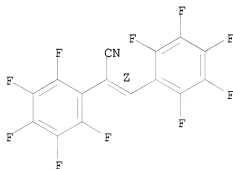
Double bond geometry as shown.





RN 25576-30-1 CAPLUS  
 CN Acrylonitrile, 2,3-bis(pentafluorophenyl)-, (Z)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.



L5 ANSWER 144 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1969:524121 CAPLUS  
 DOCUMENT NUMBER: 71:124121  
 ORIGINAL REFERENCE NO.: 71:23055a,23058a  
 TITLE: Transformations of decafluoro- $\alpha$ -phenylcinnamic acid  
 AUTHOR(S): Molosnova, V. P.; Barkhash, V. A.; Vorozhtsov, N. N., Jr.  
 CORPORATE SOURCE: Novosibirsk. Inst. Org. Khim., Novosibirsk, USSR  
 SOURCE: Zhurnal Obshchei Khimii (1969), 39(8), 1774-7  
 CODEN: ZOKHA4; ISSN: 0044-460X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 AB RMgCl from 20.8 g. C6F5Cl, prepared in N atmospheric was treated with dry CH2O over  
 30-40 min., then treated with ice-HCl to yield 73% C6F5CH2OH, b57  
 113-14.5°, m. 30-1°. C6F5CHO heated in Ac2O-Et3N with  
 C6F5CH2CO2H (prepared from above carbinol via treatment with PCl5, KCN and  
 H2O), 0.5 hr. gave after acidification a mixture of 63.6% C6F5CH:CPHCO2H  
 (I), m. 187-8°, and 2% 3-pentafluorophenyl-5,6,7,8-  
 tetrafluorocoumarin, m. 210-11°. I gave the S-benzylthiuronium  
 salt, m. 167-7.5°. I heated with KF in Me2NCHO 5 hrs. gave  
 3-pentafluorobenzylidene-4,5,6,7-tetrafluoro-2-coumarone, m.  
 185-7°, which with KMnO4 was oxidized to tetrafluorosalicic acid,  
 m. 169-70°. I and 20% oleum in CHCl3 at 40°, treated with  
 NaN3, then quenched in ice, gave 73.5% decafluorodeoxybenzoin, m.

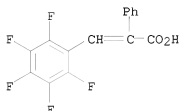
81-2°. Ir spectra were reported.

IT 1081539-52-7P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)  
(Transformations of decafluoro- $\alpha$ -phenylcinnamic acid)

RN 1081539-52-7 CAPLUS

CN Benzeneacetic acid,  $\alpha$ -[(2,3,4,5,6-pentafluorophenyl)methylene]- (CA INDEX NAME)

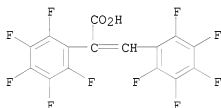


IT 24043-87-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and reactions of)

RN 24043-87-6 CAPLUS

CN Benzeneacetic acid, 2,3,4,5,6-pentafluoro- $\alpha$ -[(2,3,4,5,6-pentafluorophenyl)methylene]- (CA INDEX NAME)



IT 25955-31-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

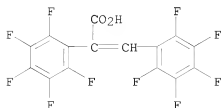
RN 25955-31-1 CAPLUS

CN Benzeneacetic acid, 2,3,4,5,6-pentafluoro- $\alpha$ -[(2,3,4,5,6-pentafluorophenyl)methylene]-, compd. with phenylmethyl carbamimidothioate (1:1) (CA INDEX NAME)

CM 1

CRN 24043-87-6

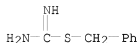
CMF C15 H2 F10 O2



CM 2

CRN 621-85-2

CMF C8 H10 N2 S



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
(3 CITINGS)

L5 ANSWER 145 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1969:403064 CAPLUS

DOCUMENT NUMBER: 71:3064

ORIGINAL REFERENCE NO.: 71:556h,557a

TITLE: Transannular interactions in tetrafluoro[2.2]paracyclophane

AUTHOR(S): Filler, Robert; Choe, E. W.

CORPORATE SOURCE: Illinois Inst. of Technol., Chicago, IL, USA

SOURCE: Journal of the American Chemical Society (1969),

91(7), 1862-4

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The Wittig reaction of BzH and C6F5CH:PPh3, prepared by treating C6F5CH2PPh3Br with BuLi, gave trans-C6F5CH:CHPh which was hydrogenated to C6F5CH2CH2Ph. H was introduced into the fluorinated ring and the product was converted to 4-formyl-2,3,5,6-tetrafluorobenzyl (I) by treatment with BuLi, followed by N-methylformanilide. Reduction of I with LiAlH4 gave the alc., which was treated with PBr3. The bromide obtained was bromomethylated to give 4,4'-bis(bromomethyl)-2,3,5,6-tetrafluorobenzyl, which was subjected to a Wurtz reaction to give 4,5,7,8-tetrafluoro[2.2]paracyclophane (II). The uv spectra of [2.2]paracyclophane, II, and octafluoro[2.2]paracyclophane were tabulated and discussed. The 1H N.M.R. spectrum of II in CC14 revealed transannular coupling between the aromatic protons of 1 ring and the F atoms of the other.

IT 19292-25-2P

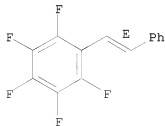
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 19292-25-2 CAPLUS

CN Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-phenylethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD

## (6 CITINGS)

L5 ANSWER 146 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1969:106077 CAPLUS

DOCUMENT NUMBER: 70:106077

ORIGINAL REFERENCE NO.: 70:19783a,19786a

TITLE: Synthesis of cis- and trans-decafluorostilbenes

AUTHOR(S): Molosnova, V. P.; Vysochin, V. I.; Barkhash, V. A.; Vorozhtsov, N. N., Jr.

CORPORATE SOURCE: Novosibirsk. Inst. Org. Khim., Novosibirsk, USSR  
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1969), (1), 146-7

CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB Heating 2.15 g. C6F5CH:C(C6F5)CO2Ag with 0.05 g. Cu chromite catalyst and 6.4 ml. dry Me2NCHO 4 hrs. at 160-5° gave after an aqueous treatment 49% mixed isomers of C6F5CH:CHC6F5 m. 50-60°, which after repeated crystallization from EtOH-petroleum ether gave the isomer m. 61-2°, which has the cis form. The more soluble isomer, m. 54-5°, also has the cis form on the basis of its spectra (uv and N.M.R.). On standing, both isomers lose the sharpness of m.p. and become approx. the same (m. 53-61°) after several months. However, no interconversion takes place during melting. C6F5CH2Br and Ph3P in C6H6 gave the quaternary salt, m. 237-9°, which with MeONa in tetrahydrofuran 2 days at room temperature under N, then treated with C6F5CHO 1 day at room temperature and 6

hrs. at reflux, gave Ph3PO and 32% trans-C6F5CH:CHC6F5, m. 101.5-3.5°.

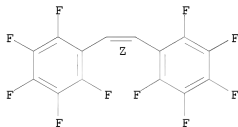
IT 14992-38-2P 14992-40-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 14992-38-2 CAPLUS

CN Benzene, 1,1'-(1Z)-1,2-ethenediylbis[2,3,4,5,6-pentafluoro- (9CI) (CA INDEX NAME)

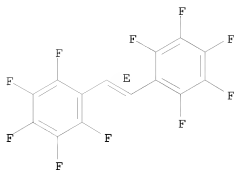
Double bond geometry as shown.



RN 14992-40-6 CAPLUS

CN Benzene, 1,1'-(1E)-1,2-ethenediylbis[2,3,4,5,6-pentafluoro- (CA INDEX NAME)

Double bond geometry as shown.



L5 ANSWER 147 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1969:67706 CAPLUS

DOCUMENT NUMBER: 70:67706

ORIGINAL REFERENCE NO.: 70:12629a,12632a

TITLE: Diels-Alder reactions of polyfluorocyclohexa-1,3-dienes. I. Addition of alkynes to perfluorocyclohexa-1,3-diene. Route to ortho-disubstituted tetrafluorobenzenes

AUTHOR(S): Anderson, Leonard Philip; Feast, William J.; Musgrave, William K. R.

CORPORATE SOURCE: Univ. Sci. Lab., Durham City, UK

SOURCE: Journal of the Chemical Society [Section] C: Organic (1969), (2), 211-17

CODEN: JSOOAX; ISSN: 0022-4952

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Perfluorocyclohexa-1,3-diene reacts with alkynes XC.tplbond.CY by 1,4-addition to give, exclusively and in good yield, 2-(X-substituted)-3-(Y-substituted)-1,4,5,6,7,7,8,8-octafluorobicyclo[2.2.2]octa-2,5-dienes (X = Y = CF<sub>3</sub>, Me, CH<sub>2</sub>Cl, CO<sub>2</sub>Et; X = H, Y = CF<sub>3</sub>, Me, CH<sub>2</sub>Cl, Ph; X = CF<sub>3</sub>, Y = Me) which eliminate tetrafluoroethylene on pyrolysis to give ortho-disubstituted tetrafluorobenzenes, or their further pyrolysis products 1-(X-substituted)-2-(Y-substituted)-3,4,5,6-tetrafluorobenzene (X = Y = CF<sub>3</sub>, Me, H; X = H, Y = CF<sub>3</sub>, Me, CH<sub>2</sub>Cl, CO<sub>2</sub>H, C.tplbond.CH, CH:CHC<sub>6</sub>H<sub>4</sub>, Ph; X = CF<sub>3</sub>, Y = Me).

IT 21651-69-4P

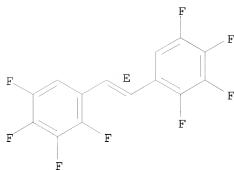
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 21651-69-4 CAPLUS

CN Benzene, 1,1'-(1,2-ethenediyl)bis[2,3,4,5-tetrafluoro-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD  
(5 CITINGS)

L5 ANSWER 148 OF 152 CAPLUS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 1968:443571 CAPLUS

DOCUMENT NUMBER: 69:43571

ORIGINAL REFERENCE NO.: 69:8147a,8150a

TITLE: Thermolysis of aromatic aldazines. IV. Similarities

and differences with electron-impact fragmentation

AUTHOR(S): Buu-Hoi, N. P.; Saaïnt-Ruf, Germain

CORPORATE SOURCE: Inst. Chim. Subst. Natur., C.N.R.S., Gif-Sur-Yvette,  
Fr.

SOURCE: Bulletin de la Societe Chimique de France (1968), (2),  
661-4

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal

LANGUAGE: French

GI For diagram(s), see printed CA Issue.

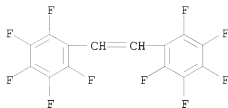
AB The thermal decomposition of aromatic aldazines was examined by mass spectrometry. Thus, 5.4 g. C<sub>6</sub>D<sub>5</sub>CHO was refluxed 3 hrs. with 1.2 g. 98% N<sub>2</sub>H<sub>4</sub>.H<sub>2</sub>O and 28 ml. EtOH to give I, m. 93°. I (5 g.) was heated at 200° till gases ceased to evolve, cooled, and distilled in vacuo to give C<sub>6</sub>D<sub>5</sub>CN (II) b. 233°, III, m. 125°, and IV, m. 275°. II, on KOH saponification gave C<sub>6</sub>D<sub>5</sub>CO<sub>2</sub>H, m. 122°. C<sub>6</sub>F<sub>5</sub>CHO (5.9 g.) was refluxed 2 hrs. with 0.75 g. N<sub>2</sub>H<sub>4</sub>.H<sub>2</sub>O in 50 ml. EtOH to give 95% pentafluorobenzaldazine (V), m. 138°. V was heated 1 hr. at 280° in paraffin oil to give C<sub>6</sub>F<sub>5</sub>CH:CHC<sub>6</sub>F<sub>5</sub> (VI), m. 101°; resolidified and remelted 158° (hexane). VI was also prepared in 50% yield by direct heating of V. The m/e, and % abundance of the fragments produced during the thermolysis of aldazines were determined. The fragmentation patterns were compared with those obtained by electronic impact techniques. A bond cleavage between the aryl group and the rest of the aldazine mol. was observed during thermolysis.

IT 19339-50-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

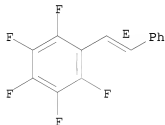
RN 19339-50-5 CAPLUS

CN Benzene, 1,1'-(1,2-ethenediyl)bis[2,3,4,5,6-pentafluoro- (CA INDEX NAME)



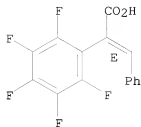
L5 ANSWER 149 OF 152 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1968:426929 CAPLUS  
 DOCUMENT NUMBER: 69:26929  
 ORIGINAL REFERENCE NO.: 69:4995a,4998a  
 TITLE: Aromatic polyfluoro compounds. XLI. Some reaction of  
 pentafluorobenzaldehyde  
 AUTHOR(S): Aroskar, E. V.; Brown, P. J. N.; Plevy, R. G.;  
 Stephens, R.  
 CORPORATE SOURCE: Univ. Birmingham, Birmingham, UK  
 SOURCE: Journal of the Chemical Society [Section] C: Organic  
 (1968), (13), 1569-75  
 CODEN: JSOQAX; ISSN: 0022-4952  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI For diagram(s), see printed CA Issue.  
 AB Pentafluorobenzaldehyde was converted into a range of derivs. by reactions  
 involving the carbonyl group, viz., a pentafluorostilbene, a  
 pentafluorocinnamic acid (I), an azine, an oxime, and a range of acetals.  
 Other derivs., e.g. II, were made by reactions involving replacement of F  
 using Me<sub>2</sub>NH, NaHS, PhSNa, and NaOMe.  
 IT 19292-25-2P 19292-26-3P 19573-98-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 19292-25-2 CAPLUS  
 CN Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-phenylethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 19292-26-3 CAPLUS  
 CN Acrylic acid, 2-(pentafluorophenyl)-3-phenyl-, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.

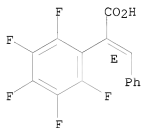


RN 19573-98-9 CAPLUS  
 CN Acrylic acid, 2-(pentafluorophenyl)-3-phenyl-, compd. with  
 2-benzyl-2-thiopseudourea (1:1), (E)- (8CI) (CA INDEX NAME)

CM 1

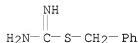
CRN 19292-26-3  
 CMF C15 H7 F5 O2

Double bond geometry as shown.



CM 2

CRN 621-85-2  
 CMF C8 H10 N2 S



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS  
 RECORD (11 CITINGS)

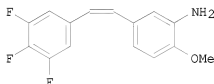
=> s l5 and cancer  
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 L6 0 L5 AND CANCER

=> s l5 and cancer  
 414531 CANCER  
 60981 CANCERS  
 429588 CANCER  
 (CANCER OR CANCERS)  
 L7 3 L5 AND CANCER

=> d ibib abs tot



L7 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2008:1136076 CAPLUS  
 DOCUMENT NUMBER: 149:533971  
 TITLE: Design, synthesis, biochemical, and biological  
 evaluation of nitrogen-containing trifluoro structural  
 modifications of combretastatin A-4  
 AUTHOR(S): Hall, John J.; Sriram, Madhavi; Strecker, Tracy E.;  
 Tidmore, Justin K.; Jelinek, Christopher J.; Kumar, G.  
 D. Kishore; Hadimani, Mallinath B.; Pettit, George R.;  
 Chaplin, David J.; Trawick, Mary Lynn; Pinney, Kevin  
 G.  
 CORPORATE SOURCE: Department of Chemistry and Biochemistry, Baylor  
 University, Waco, TX, 76798-7348, USA  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2008),  
 18(18), 5146-5149  
 CODEN: BMCLE8; ISSN: 0960-894X  
 PUBLISHER: Elsevier Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 149:533971  
 GI



I

AB A new trifluorinated amino-combretastatin analog,  
 (Z)-2-(4'-methoxy-3'-aminophenyl)-1-(3,4,5-trifluorophenyl)ethene (I),  
 prepared by chemical synthesis, was found to be a potent inhibitor of tubulin  
 assembly (IC50 = 2.9  $\mu$ M), and cytotoxic against selected human  
 cancer cell lines. This new lead compound is among the most active  
 from a group of related structural modifications.  
 OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
 (1 CITINGS)  
 REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2004:754412 CAPLUS  
 DOCUMENT NUMBER: 141:277352  
 TITLE: Preparation of quinone and catechol derivatives for  
 the treatment of cancers and other vascular  
 proliferative disorders  
 INVENTOR(S): Chaplin, David J.; Edvardsen, Klaus; Pinney, Kevin G.;  
 Prezioso, Joseph Anthony; Wood, Mark  
 PATENT ASSIGNEE(S): Oxigene, Inc., USA  
 SOURCE: PCT Int. Appl., 101 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004078126	A2	20040916	WO 2004-US6175	20040301
WO 2004078126	A3	20050811		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI

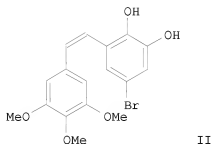
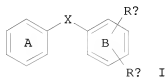
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2004218412	A1	20040916	AU 2004-218412	20040301
CA 2516078	A1	20040916	CA 2004-2516078	20040301
EP 1601348	A2	20051207	EP 2004-716108	20040301

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PRIORITY APPLN. INFO.:  
 US 2003-450565P P 20030228  
 US 2003-467486P P 20030502  
 WO 2004-US6175 A 20040301

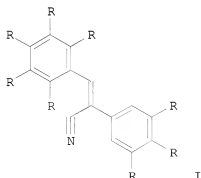
OTHER SOURCE(S): CASREACT 141:277352; MARPAT 141:277352  
 GI



AB The title compound I [Ring A is optionally substituted with one to five substituents selected from alkoxy, cycloalkoxy, halo, trihaloalkyl, alkyl, allyl, alc., (substituted)amino, oxo, alkanoyl, thiol, etc.; ring B comprises at least one structure denoted by Ra and Rb which represent an ortho-quinone (-CO-CO-), or ortho-catechol (-COH-COH-) or ortho-catechol pro-drug moiety; the remaining carbons of B ring are optionally substituted with one to five substituents selected from alkoxy, cycloalkoxy, halo, trihaloalkyl, alkyl, allyl, alc., (substituted)amino, oxo, alkanoyl, thiol, etc.; Bridge X = alkene, alkane, alkyne, amide, amine, etc.] were prepared for the treatment of solid tumor cancers and other vascular proliferative disorders. For example, compound II was prepared in a multi-step synthesis starting from 5-bromo-2-hydroxy-3-methoxybenzaldehyde. The latter showed activity with IC50s of 2.1 and 0.34  $\mu$ M in the tubulin binding and MTT assays.

TITLE: Breast cancer resistance protein (BCRP) inhibitor  
 INVENTOR(S): Yamazaki, Ryuta; Nishiyama, Yukiko; Furuta, Tomio; Matsuzaki, Takeshi; Hatano, Hiroshi; Yoshida, Oh; Nagaoka, Masato; Aiyama, Ritsuo; Hashimoto, Shusuke; Sugimoto, Yoshikazu  
 PATENT ASSIGNEE(S): Kabushiki Kaisha Yakult Honsha, Japan  
 SOURCE: PCT Int. Appl., 91 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004069243	A1	20040819	WO 2004-JP1067	20040203
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG				
AU 2004210259	A1	20040819	AU 2004-210259	20040203
AU 2004210259	B2	20081211		
CA 2515174	A1	20040819	CA 2004-2515174	20040203
EP 1591117	A1	20051102	EP 2004-707629	20040203
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2004007264	A	20060131	BR 2004-7264	20040203
CN 1744892	A	20060308	CN 2004-80003247	20040203
ZA 2005005988	A	20061227	ZA 2005-5988	20050726
IN 2005DN03346	A	20070413	IN 2005-DN3346	20050727
US 20060128636	A1	20060615	US 2005-544064	20050802
US 7371773	B2	20080513		
MX 2005008298	A	20050920	MX 2005-8298	20050804
NO 2005003956	A	20051026	NO 2005-3956	20050825
PRIORITY APPLN. INFO.:			JP 2003-26856	A 20030204
			WO 2004-JP1067	W 20040203
OTHER SOURCE(S):		MARPAT 141:200160		
GI				



AB A drug which inhibits BCRPs. It is a breast cancer resistance

protein inhibitor which contains as an active ingredient either a diphenylacrylonitrile derivative represented by the following formula (I): (I) {wherein the eight R's are the same or different and each independently represents hydrogen, hydroxy, nitro, amino, acetylamino (-NHCOCH3), cyano (-CN), formyl (-CHO), -COOR1 (R1 is hydrogen or C1-4 alkyl), -O(CH2)nCOOR2 (n is 1 to 7 and R2 is hydrogen or C1-4 alkyl), -OOCH2CH2COOR3 (R3 is hydrogen, C1-4 alkyl, (Z)-2-(3,4-dimethoxyphenyl)-3-(4-hydroxyphenyl)acrylonitrile, or glycopyranosyl), C1-8 alkoxy, C1-4 alkyl, halogeno, ((C1-4 alkoxy)C1-4 alkoxy)C1-4 alkoxy, C2-8 acyloxy, C2-8 halogenoacyloxy, methylenedioxy, trifluoromethyl, phosphate group (-OP(O)(OH)2) or salt thereof, sulfate group (-OSO3H) or salt thereof, glycopyranosyl or salt thereof, a glycopyranosyl phosphate or salt thereof, glycopyranosyl sulfate or salt thereof, or piperidinopiperidinocarbonyloxy} or an ester or salt of the derivative

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>  
=> s 15 not py>2003  
7570071 PY>2003  
L8 96 L5 NOT PY>2003

=> focus  
PROCESSING COMPLETED FOR L8  
L9 96 FOCUS L8 1-

=> d ibib abs hitstr

L9 ANSWER 1 OF 96 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1987:458571 CAPLUS

DOCUMENT NUMBER: 107:58571

ORIGINAL REFERENCE NO.: 107:9717a,9720a

TITLE: Application of organoelement compounds of the fifth and sixth groups in organic synthesis. Part 44. A facile synthesis of pentafluorophenyl olefins via an arsonium ylide

AUTHOR(S): Shen, Yanchang; Qiu, Weiming

CORPORATE SOURCE: Shanghai Inst. Org. Chem., Acad. Sin., Shanghai, Peop. Rep. China

SOURCE: Synthesis (1987), (1), 65-6  
CODEN: SYNTBF; ISSN: 0039-7881

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 107:58571

AB Benzaldehydes were treated with C6F5CH:AsPh3(I) to give C6F5CH:CHR1 (R1 = Ph, halophenyl, O2NC6H4, anisyl, styryl, etc.). I was obtained from CH2:AsPh3 and C6F6.

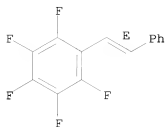
IT 19292-25-2P 37516-14-6P 37516-15-7P  
78622-66-9P 109384-55-6P 109384-56-7P  
109384-57-8P 109384-58-9P 109384-59-0P  
109384-60-3P 109384-61-4P 109384-62-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 19292-25-2 CAPLUS

CN Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-phenylethenyl]- (CA INDEX NAME)

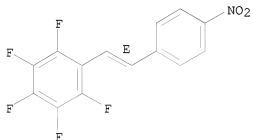
Double bond geometry as shown.



RN 37516-14-6 CAPLUS

CN Benzene, pentafluoro[(1E)-2-(4-nitrophenyl)ethenyl]- (9CI) (CA INDEX NAME)

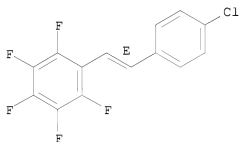
Double bond geometry as shown.



RN 37516-15-7 CAPLUS

CN Benzene, [(1E)-2-(4-chlorophenyl)ethenyl]pentafluoro- (9CI) (CA INDEX NAME)

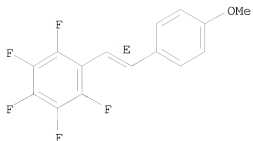
Double bond geometry as shown.



RN 78622-66-9 CAPLUS

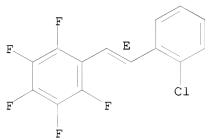
CN Benzene, 1,2,3,4,5-pentafluoro-6-[(1E)-2-(4-methoxyphenyl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



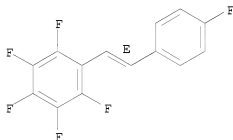
RN 109384-55-6 CAPLUS  
 CN Benzene, [(1E)-2-(2-chlorophenyl)ethenyl]pentafluoro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



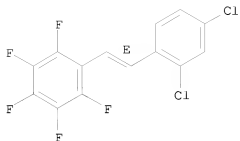
RN 109384-56-7 CAPLUS  
 CN Benzene, pentafluoro[2-(4-fluorophenyl)ethenyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



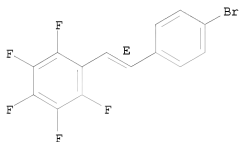
RN 109384-57-8 CAPLUS  
 CN Benzene, [2-(2,4-dichlorophenyl)ethenyl]pentafluoro-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



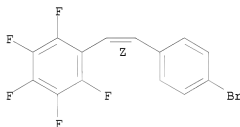
RN 109384-58-9 CAPLUS  
 CN Benzene, 1-[(1E)-2-(4-bromophenyl)ethenyl]-2,3,4,5,6-pentafluoro- (CA INDEX NAME)

Double bond geometry as shown.



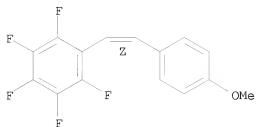
RN 109384-59-0 CAPLUS  
 CN Benzene, [2-(4-bromophenyl)ethenyl]pentafluoro-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



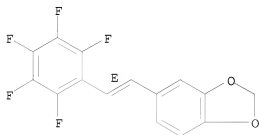
RN 109384-60-3 CAPLUS  
 CN Benzene, pentafluoro[2-(4-methoxyphenyl)ethenyl]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



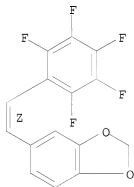
RN 109384-61-4 CAPLUS  
 CN 1,3-Benzodioxole, 5-[2-(pentafluorophenyl)ethenyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 109384-62-5 CAPLUS  
 CN 1,3-Benzodioxole, 5-[2-(pentafluorophenyl)ethenyl]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



=> fil reg  
 COST IN U.S. DOLLARS  
 FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
115.58	310.06

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  
 CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
-13.94	-13.94



FILE 'REGISTRY' ENTERED AT 10:10:42 ON 29 JUL 2009  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2009 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 27 JUL 2009 HIGHEST RN 1169753-75-6  
DICTIONARY FILE UPDATES: 27 JUL 2009 HIGHEST RN 1169753-75-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

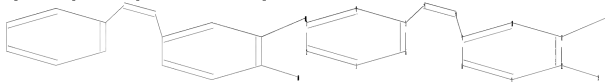
Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10-790662 -b.str



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chain nodes :  
13 14 15 16  
ring nodes :  
1 2 3 4 5 6 7 8 9 10 11 12  
chain bonds :  
5-13 9-14 11-16 12-15 13-14  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12  
exact/norm bonds :  
11-16 12-15  
exact bonds :  
5-13 9-14 13-14  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
```

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS

=> d  
 L10 HAS NO ANSWERS  
 L10 STR



Structure attributes must be viewed using STN Express query preparation.

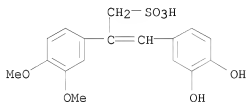
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 SAMPLE SEARCH INITIATED 10:11:16 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 787 TO ITERATE  
 100.0% PROCESSED 787 ITERATIONS 22 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 14057 TO 17423  
 PROJECTED ANSWERS: 159 TO 721

L11 22 SEA SSS SAM L10

=> d scan

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenesulfonic acid,  $\beta$ -[(3,4-dihydroxyphenyl)methylene]-3,4-  
 dimethoxy-  
 MF C17 H18 O7 S

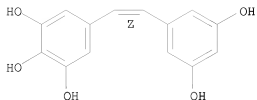


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):21

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 1,2,3-Benzenetriol, 5-[2-(3,5-dihydroxyphenyl)ethenyl]-, (Z)- (9CI)  
 MF C14 H12 O5

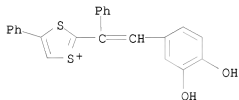
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 1,3-Dithiol-1-ium, 2-[2-(3,4-dihydroxyphenyl)-1-phenylethenyl]-4-phenyl-,  
 perchlorate (1:1)  
 MF C23 H17 O2 S2 . C1 O4

CM 1

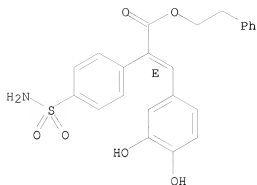


CM 2



L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetic acid, 4-(aminosulfonyl)- $\alpha$ -[(3,4-  
 dihydroxyphenyl)methylene]-, 2-phenylethyl ester, ( $\alpha$ E)-  
 MF C23 H21 N O6 S

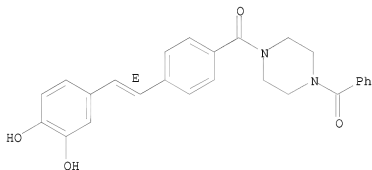
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Methanone, (4-benzoyl-1-piperazinyl)[4-[(1E)-2-(3,4-  
 MF C26 H24 N2 O4  
 dihydroxyphenyl)ethenyl]phenyl]-

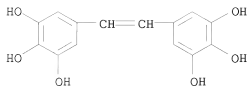
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

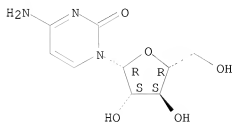
L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 2(1H)-Pyrimidinone, 4-amino-1-β-D-arabinofuranosyl-, mixt. with  
 5,5'-(1,2-ethenediyl)bis[1,2,3-benzenetriol] (9CI)  
 MF C14 H12 O6 . C9 H13 N3 O5  
 CI MXS

CM 1



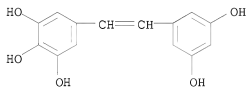
CM 2

Absolute stereochemistry.



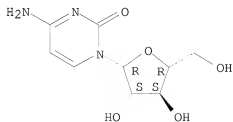
L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 2(1H)-Pyrimidinone, 4-amino-1-β-D-arabinofuranosyl-, mixt. with  
 5-[2-(3,5-dihydroxyphenyl)ethenyl]-1,2,3-benzenetriol (9CI)  
 MF C14 H12 O5 . C9 H13 N3 O5  
 CI MXS

CM 1

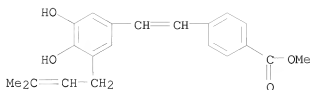


CM 2

Absolute stereochemistry.

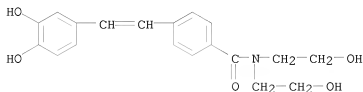


L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzoic acid, 4-[2-[3,4-dihydroxy-5-(3-methyl-2-buten-1-yl)phenyl]ethenyl]-  
 , methyl ester  
 MF C21 H22 O4



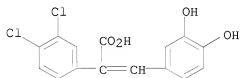
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzamide, 4-[2-(3,4-dihydroxyphenyl)ethenyl]-N,N-bis(2-hydroxyethyl)-  
 MF C19 H21 N O5



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

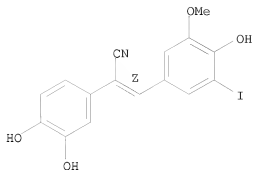
L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetic acid, 3,4-dichloro- $\alpha$ -[(3,4-dihydroxyphenyl)methylene]-  
 MF C15 H10 Cl2 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

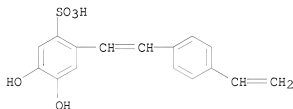
L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile, 3,4-dihydroxy- $\alpha$ -[(4-hydroxy-3-iodo-5-methoxyphenyl)methylene]-, ( $\alpha$ Z)-  
 MF C16 H12 I N O4

Double bond geometry as shown.



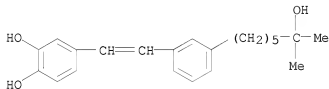
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenesulfonic acid, 2-[2-(4-ethenylphenyl)ethenyl]-4,5-dihydroxy-  
 MF C16 H14 O5 S  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 1,2-Benzenediol, 4-[2-[3-(6-hydroxy-6-methylheptyl)phenyl]ethenyl]-  
 MF C22 H28 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

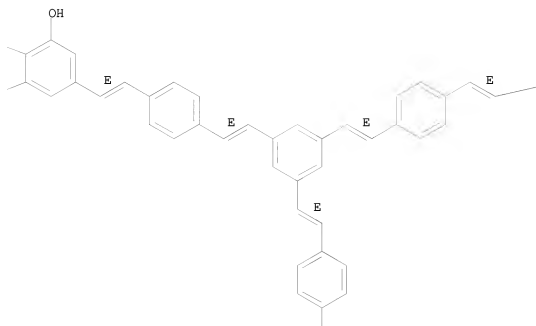
L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 1,2,3-Benzenetriol, 5,5',5'',5''',5''''',5''''''-[1,3,5-benzenetriyltris[(1E)-2,1-ethenediyl-4,1-phenylene-(1E)-2,1-ethenediyl-5,1,3-benzenetriylbis[(1E)-2,1-ethenediyl-4,1-phenylene-(1E)-2,1-ethenediyl]]]hexakis- (9CI)  
 MF C150 H114 O18

Double bond geometry as shown.

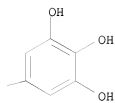
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PAGE 1-B

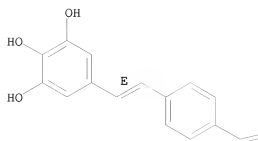


PAGE 1-C

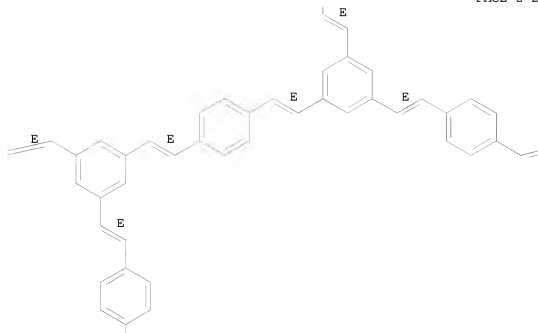




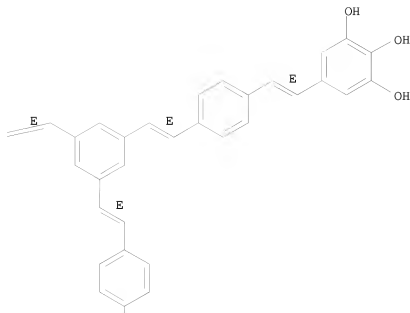
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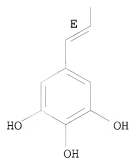
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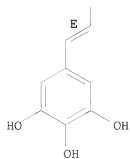
PAGE 2-C



PAGE 3-B

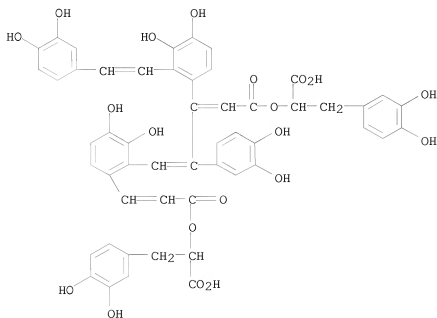


PAGE 3-C



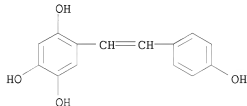
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzenepropanoic acid,  $\alpha$ -[3-[2-[5-[1-carboxy-2-(3,4-dihydroxyphenyl)ethoxy]-2-(3,4-dihydroxyphenyl)-3-[2-[2-(3,4-dihydroxyphenyl)ethenyl]-3,4-dihydroxyphenyl]-5-oxo-1,3-pentadien-1-yl]-3,4-dihydroxyphenyl]-1-oxo-2-propen-1-yl]oxy]-3,4-dihydroxy-  
 MF C52 H42 O20



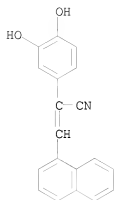
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 1,2,4-Benzenetriol, 5-[2-(4-hydroxyphenyl)ethenyl]-  
 MF C14 H12 O4



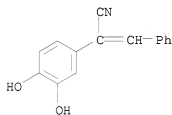
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile, 3,4-dihydroxy- $\alpha$ -(1-naphthalenylmethylene)-  
 MF C19 H13 N O2



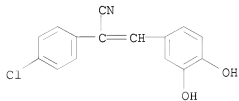
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile, 3,4-dihydroxy- $\alpha$ -(phenylmethylene)-  
 MF C15 H11 N O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

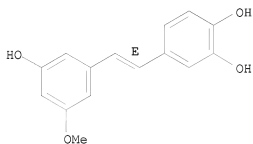
L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN Benzeneacetonitrile, 4-chloro- $\alpha$ -[(3,4-dihydroxyphenyl)methylene]-  
 MF C15 H10 Cl N O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

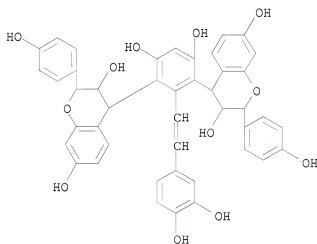
L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 1,2-Benzenediol, 4-[(1E)-2-(3-hydroxy-5-methoxyphenyl)ethenyl]-  
 MF C15 H14 O4

Double bond geometry as shown.



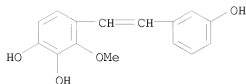
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 2H-1-Benzopyran-3,7-diol, 4,4'-[2-[2-(3,4-dihydroxyphenyl)ethenyl]-4,6-dihydroxy-1,3-phenylene]bis[3,4-dihydro-2-(4-hydroxyphenyl)-, [2R-[2 $\alpha$ ,3 $\alpha$ ,4 $\beta$ [(2'R\*,3'S\*,4'S\*)]]]- (9CI)  
 MF C44 H36 O12



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 22 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN 1,2-Benzenediol, 4-[2-(3-hydroxyphenyl)ethenyl]-3-methoxy-  
 MF C15 H14 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> s l10 full

FULL SEARCH INITIATED 10:11:39 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 15465 TO ITERATE

100.0% PROCESSED 15465 ITERATIONS

412 ANSWERS

SEARCH TIME: 00.00.01

L12 412 SEA SSS FUL L10

=> fil capl

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

186.36

496.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

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FILE COVERS 1907 - 29 Jul 2009 VOL 151 ISS 5

FILE LAST UPDATED: 28 Jul 2009 (20090728/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/CAPLUS family of databases have been updated to include new citing references information. This enhancement may impact record import into database management software. For additional information, refer to NEWS 22.

=> s l12

L13 1181 L12

=> a l13 and cancer

A IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.

For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> s l13 and cancer

414531 CANCER

60981 CANCERS

429588 CANCER

(CANCER OR CANCERS)

L14 111 L13 AND CANCER

=> s l14 not py>2002

8578358 PY>2002

L15 26 L14 NOT PY>2002

=> d ibib abs 25-26 hitstr

L15 ANSWER 25 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1987:451278 CAPLUS

DOCUMENT NUMBER: 107:51278

ORIGINAL REFERENCE NO.: 107:8347a,8350a

TITLE: Analysis of tamoxifen and its metabolites in human plasma by gas chromatography-mass spectrometry (GC-MS) using selected ion monitoring (SIM)

AUTHOR(S): Murphy, C.; Fotsis, T.; Pantzar, P.; Adlercreutz, H.; Martin, F.

CORPORATE SOURCE: Dep. Pharmacol., Univ. Coll. Dublin, Dublin, Ire.

SOURCE: Journal of Steroid Biochemistry (1987), 26(5), 547-55  
CODEN: JSTBBK; ISSN: 0022-4731

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A method for the anal. of tamoxifen and its metabolites in the plasma from tamoxifen-treated breast cancer patients, by capillary GC-MS using selected ion monitoring, is described. Metabolite extraction was carried out on a Sep-pak C18 cartridge and metabolite purification by selective ion-exchange chromatog. steps. Satisfactory recovery of radioactive stds. through the extraction and purification steps was obtained. The method was accurate

and precise with precision coefficient of variation values ranging from 4.3-11% for tamoxifen and its metabolites. Tamoxifen, 4-hydroxytamoxifen, metabolite Y and N-desmethyltamoxifen were identified with certainty in the plasma on the basis of GC relative retention times and mass spectral comparison with authentic stds.; because of their low abundance in the plasma cis-metabolite E and 3,4-dihydroxytamoxifen could only be tentatively identified but identical GC behavior and a satisfactory comparison of the abundance of key fragment ions was achieved. The tamoxifen and metabolite concentration ranges (ng/mL) in the group of patients who received 40 or 80 ng tamoxifen for 14 days were tamoxifen, 307-745;

N-desmethyltamoxifen, 185-491; 4-hydroxytamoxifen, 1.4-2.5;  
3,4-dihydroxytamoxifen, 0.7-2.0; metabolite Y, 19.0-112; and metabolite  
E1, 0.9-2.0.

IT 81992-84-9, 3,4-Dihydroxytamoxifen

RL: ANT (Analyte); ANST (Analytical study)

(determination of, in blood plasma of humans, as tamoxifen metabolite, by

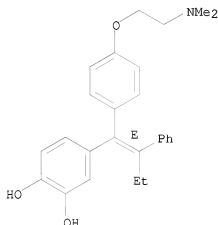
gas

chromatog.-mass spectrometry)

RN 81992-84-9 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-  
buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS  
RECORD (12 CITINGS)

L15 ANSWER 26 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1987:44185 CAPLUS

DOCUMENT NUMBER: 106:44185

ORIGINAL REFERENCE NO.: 106:7209a,7212a

TITLE: Calmodulin antagonism and growth-inhibiting activity  
of triphenylethylene antiestrogens in MCF-7 human  
breast cancer cells

AUTHOR(S): Gulino, Alberto; Barrera, Giuseppina; Vacca,  
Alessandra; Farina, Antonietta; Ferretti, Carlo;  
Screpanti, Isabella; Dianzani, Mario U.; Frati, Luigi  
CORPORATE SOURCE: Dip. Med. Sper., Univ. "La Sapienza", Rome, 00161,  
Italy

SOURCE: Cancer Research (1986), 46(12, Pt. 1), 6274-8

CODEN: CNREA8; ISSN: 0008-5472

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The effects of the triphenylethylene antiestrogens tamoxifen  
[10540-29-1], N-demethyltamoxifen [31750-48-8], nafoxidine [1845-11-0],  
hydroxytamoxifen [68047-06-3], and 3,4-dihydroxytamoxifen [  
81992-84-9] on the inhibition of both calmodulin-dependent cAMP  
phosphodiesterase [9036-21-9] activity and proliferation of breast  
cancer cells (MCF-7) were studied. Hydroxylation of the  
triphenylethylene mol. decreased its ability to inhibit  
calmodulin-dependent phosphodiesterase activity in vitro. Furthermore,  
the growth-inhibiting activity of several antiestrogens and other  
calmodulin antagonists [R24571 [57265-65-3], trifluoperazine [117-89-5],  
N-(6-aminoheptyl)-5-chloronaphthalene-1-sulfonamide [65595-90-6], and



N-(6-aminoethyl)-1-naphthalenesulfonamide [79458-81-4]] correlated with their antagonistic effects on calmodulin activity. The level of activity was: R24571 > tamoxifen = N-demethyltamoxifen = nafoxidine > 4-hydroxytamoxifen > 3,4-dihydroxytamoxifen = trifluoperazine > N-(6-aminoethyl)-5-chloronaphthalene-1-sulfonamide > metabolite A > N-(6-aminoethyl)-1-naphthalenesulfonamide. However, the protein kinase C-activating and -inhibiting drugs (phorbol tetradecanoate 13-acetate and tamoxifen, resp.) had a synergistic inhibitory effect on MCF-7 cell growth. Thus, antiestrogen interactions with calmodulin, and not protein kinase C, may play a role in mediating the drug induced estrogen-independent inhibition of breast cancer cell growth.

IT 81992-84-9, 3,4-Dihydroxytamoxifen

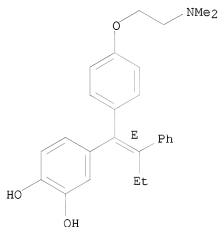
RL: BIOL (Biological study)

(mammary gland neoplasm growth inhibition by, of human, calmodulin antagonism mediation of)

RN 81992-84-9 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINGS)

=> d ibib abs hitstr 20-24

L15 ANSWER 20 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:169742 CAPLUS

DOCUMENT NUMBER: 130:346830

TITLE: The aromatase inactivator 4-hydroxyandrostenedione (4-OH-A) inhibits tamoxifen metabolism by rat hepatic cytochrome P-450 3A: potential for drug-drug interaction of tamoxifen and 4-OH-A in combined anti-breast cancer therapy

AUTHOR(S): Dehal, Shangara S.; Brodie, Angela M. H.; Kupfer, David

CORPORATE SOURCE: Department of Pharmacology and Molecular Toxicology, University of Massachusetts Medical Center, Worcester, MA, USA

SOURCE: Drug Metabolism and Disposition (1999), 27(3), 389-394 CODEN: DMSAI; ISSN: 0090-9556

PUBLISHER: American Society for Pharmacology and Experimental Therapeutics

DOCUMENT TYPE: Journal  
LANGUAGE: English

AB Tamoxifen (tam), an anti-breast cancer agent, is metabolized into tam-N-oxide by the hepatic flavin-containing monooxygenase and into N-desmethyl- and 4-hydroxy-tam by cytochrome P-450s (CYPs). Addnl., tam is metabolically activated by hepatic CYP3A, forming a reactive intermediate that binds covalently to proteins. Tam and 4-hydroxyandrostenedione (4-OH-A) are currently used to treat breast cancer, and it has been contemplated that 4-OH-A be given concurrently with tam to contravene potential tumor resistance to tam. Because alterations in tam metabolism may influence its therapeutic efficacy, the effect of 4-OH-A on tam metabolism was examined. Incubation of tam with liver microsomes from phenobarbital-treated rats, in the presence of 4-OH-A (10-100  $\mu$ M), resulted in marked inhibition of tam-N-demethylation and tam covalent binding and in decreased tam-N-oxide accumulation; however, there was no inhibition of the formation of 4-hydroxy-tam and of 3,4-dihydroxytamoxifen. These findings indicate that 4-OH-A inhibits CYP3A, but not P 450(s) that catalyze tam 4-hydroxylation. The diminished tam-N-oxide accumulation could be due to decreased N-oxide formation and/or due to increased N-oxide reduction. Incubation of tam-N-oxide with liver microsomes containing heat-inactivated flavin-containing

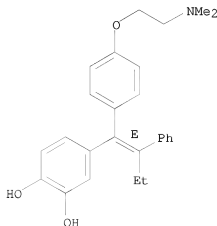
monooxygenase demonstrated that 4-OH-A increases the accumulation of tam, possibly by diminishing its P 450-mediated metabolism. Kinetic studies indicate that 4-OH-A is a competitive inhibitor of CYP3A, but not a time-dependent inactivator. Consequently, the concurrent treatment of tam and 4-OH-A may result in increased tam half-life and thus could potentiate the therapeutic efficacy of tam and diminish the potential side effects of tam by inhibiting its covalent binding to proteins and possibly to DNA.

IT 81992-84-9, 3,4-Dihydroxytamoxifen  
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)  
(4-hydroxyandrostenedioneinhibits tamoxifen metabolism by rat hepatic cytochrome P 450 3A and potential for drug-drug interaction in combined anti-breast cancer therapy)

RN 81992-84-9 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS

## RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 21 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:277674 CAPLUS

DOCUMENT NUMBER: 129:49604

ORIGINAL REFERENCE NO.: 129:10215a,10218a

TITLE: Evaluation of the antioxidant potential of natural products

AUTHOR(S): Lee, Sang Kook; Mwambo, Zakaria H.; Chung, HaSook; Luyengi, Lumonadio; Gamez, Esperanza J. C.; Mehta, Rajendra G.; Kinghorn, A. Douglas; Pezzuto, John M.

CORPORATE SOURCE: Program for Collaborative Research in the Pharmaceutical Sciences, and Department of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, University of Illinois, Chicago, IL, 60612, USA

SOURCE: Combinatorial Chemistry and High Throughput Screening (1998), 1(1), 35-46

CODEN: CCHSFU; ISSN: 1386-2073

PUBLISHER: Bentham Science Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Since reactive oxygen radicals play an important role in carcinogenesis and other human disease states, antioxidants present in consumable fruits, vegetables, and beverages have received considerable attention as cancer chemopreventive agents. Thus, in order to identify antioxidants in plant exts., test materials were assessed for potential to scavenge stable 1,2-diphenyl-2-picrylhydrazyl (DPPH) free radicals, reduce TPA-induced free radical formation in cultured HL-60 human leukemia cells, and inhibit responses observed with a xanthine/xanthine oxidase assay system. Approx. 700 plant exts. were evaluated, and 28 were found to be active in the DPPH free radical scavenging assay. Based on secondary analyses performed to assess inhibition of 7,12-dimethylbenz(a)anthracene-induced preneoplastic lesion formation with a mouse mammary organ culture model, *Chorizanthe diffusa* Benth. (Polygonaceae), *Mezoneuron cucullatum* Roxb. (Leguminosae), *Cerbera manghas* L. (Apocynaceae) and *Daphniphyllum calycinum* Benth. (Daphniphyllaceae) were selected and subjected to bioassay-guided fractionation. 5,7,3',5',-Tetrahydroxy-8,4'-dimethoxyflavonol, 5,8,4'-trihydroxy-7,3'-dimethoxyflavonol, 5,3',4'-trihydroxy-7-methoxyflavonol, and 6,3',4'-trihydroxy-7-methoxyflavonol were identified as active principles from *C. diffusa*. Piceatannol, trans-resveratrol, apigenin and scirpusin A were found as the active principles of *M. cucullatum*, olivil, (-)-carinol, and (+)-cycloolivil were active principles from *C. manghas*, and 5,6,7,4'-tetrahydroxyflavone 3-o-rutinoside and kaempferol 3-o-neohesperidoside were active principles from *D. calycinum*. Of these substances, the hydroxystilbenes piceatannol and trans-resveratrol have thus far been shown to inhibit carcinogen-induced preneoplastic lesion formation in the mouse mammary gland organ culture model.

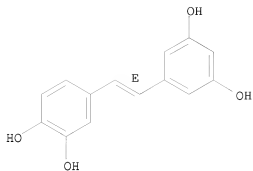
IT 10083-24-6, Piceatannol

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
(antioxidant potential of natural products)

RN 10083-24-6 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-2-(3,5-dihydroxyphenyl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 108 THERE ARE 108 CAPLUS RECORDS THAT CITE THIS RECORD (108 CITINGS)  
 REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 22 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:155442 CAPLUS

DOCUMENT NUMBER: 124:251181

ORIGINAL REFERENCE NO.: 124:46277a, 46280a

TITLE: Evidence that the catechol 3,4-dihydroxytamoxifen is a proximate intermediate to the reactive species binding covalently to proteins

AUTHOR(S): Dehal, Shangara S.; Kupfer, David  
 CORPORATE SOURCE: Worcester Foundation for Biomedical Research, Shrewsbury, MA, 01545, USA

SOURCE: Cancer Research (1996), 56(6), 1283-90  
 CODEN: CNREAB; ISSN: 0008-5472

PUBLISHER: American Association for Cancer Research

DOCUMENT TYPE: Journal

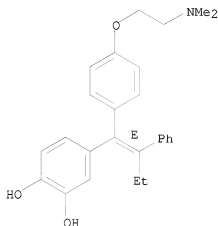
LANGUAGE: English

AB Metabolism of tamoxifen by rat and human hepatic microsomal cytochrome P450s (CYPs) forms a reactive intermediate that irreversibly binds to microsomal proteins (C. Mani and D. Kupfer, Cancer Res., 51: 6052-6058, 1991). The current study examines intermediate(s). The rate of covalent binding of tamoxifen metabolites, tamoxifen N-oxide, N-desmethyltamoxifen, and tamoxifen N-oxide-epoxide was approx. equal to or less than that of tamoxifen. By contrast, covalent binding of 4-hydroxytamoxifen (3-OH-tam) was 3-5-fold higher than that of tamoxifen, indicating that among the metabolites examined, 4-OH-tam or its metabolite(s) is most proximate to the reactive intermediate(s). Incubations of 4-OH-tam with liver microsomes from PCN-treated rats yielded three detectable metabolites. One was identified as 4-OH-tam N-oxide via its facile reduction back to 4-OH-tam by titanium(III) chloride. Another metabolite of 4-OH-tam, assumed to be 3,4-dihydroxytamoxifen (3,4-di-OH-tam) catechol, was demonstrated by its monomethylation with [3H]S-adenosyl-L-methionine ([3H]SAM) in the presence of endogenous catechol-O-methyltransferase. Monomethylated catechol from 4-OH-tam was formed at a 3-4-fold higher rate than from tamoxifen. It was reasoned that if the catechol is the most proximate metabolite to the reactive intermediate, then its methylation would reduce the formation of the reactive intermediate and result in a lower rate of covalent binding. In fact, addition of radio-inert SAM to incubations of tamoxifen inhibited covalent binding by 17-23%. By contrast, inclusion of 1.0 mM S-adenosyl-L-homocysteine, a potent inhibitor of catechol-O-methyltransferase-mediated methylation of 3,4-di-OH-tam, essentially overcame the inhibition of the covalent binding by SAM. Adnl., ascorbic acid and glutathione, inhibitors of covalent binding of tamoxifen, produced an elevation of methylated catechol. These findings

collectively indicate that 3,4-di-OH-tam is proximate to the ultimate reactive intermediate that results in covalent binding to microsomal proteins.

IT 81992-84-9, 3,4-Dihydroxytamoxifen  
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)  
(3,4-dihydroxytamoxifen is the tamoxifen metabolite proximate to the reactive intermediate that results in protein binding)  
RN 81992-84-9 CAPLUS  
CN 1,2-Benzenediol, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 43 THERE ARE 43 CAPLUS RECORDS THAT CITE THIS RECORD (43 CITINGS)

L15 ANSWER 23 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:289266 CAPLUS

DOCUMENT NUMBER: 120:289266

ORIGINAL REFERENCE NO.: 120:50679a,50682a

TITLE: Analysis of phase I and phase II metabolites of

tamoxifen in breast cancer patients

AUTHOR(S): Poon, G. K.; Chui, Y. C.; McCague, R.; Loenning, P.

E.; Feng, R.; Rowlands, M. G.; Jarman, M.

CORPORATE SOURCE: Drug Dev. Sect., Inst. Cancer Res.,

Belmont/Sutton/Surrey, SM2 5NG, UK

SOURCE: Drug Metabolism and Disposition (1993), 21(6), 1119-24

CODEN: DMSDAI; ISSN: 0090-9556

DOCUMENT TYPE: Journal

LANGUAGE: English

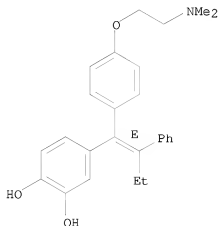
AB This study describes the application of LC/MS/MS to the determination of phase

I

and phase II metabolites of tamoxifen in urine and plasma samples of breast cancer patients. In the plasma exts., in addition to the parent drug and N-desmethyltamoxifen, a minor metabolite tamoxifen N-oxide was identified for the first time in human. Four intact glucuronides of tamoxifen metabolites were isolated in the 24-h posttreatment urine sample. They were the glucuronides of 4-hydroxytamoxifen, 4-hydroxy-N-desmethyltamoxifen, dihydroxytamoxifen, and a monohydroxy-N-desmethyltamoxifen. Hydroxylation followed by glucuronidation is a well-estimated metabolic route of tamoxifen, and this study describes for the first time direct analyses of these metabolites in human urine samples using online LC tandem MS.

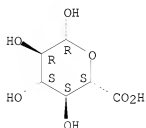
IT 155144-62-0  
 RL: ANT (Analyte); ANST (Analytical study)  
 (determination of, as metabolite, in blood plasma and urine of humans with  
 breast cancer, by HPLC-mass spectrometry)  
 RN 155144-62-0 CAPLUS  
 CN  $\beta$ -D-Glucopyranosiduronic acid, 4(or  
 5)-[1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2-  
 hydroxyphenyl, (E)- (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 81992-84-9  
 CMF C26 H29 N O3

Double bond geometry as shown.



CM 2  
 CRN 23018-83-9  
 CMF C6 H10 O7

Absolute stereochemistry.

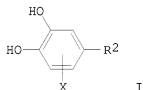


OS.CITING REF COUNT: 49 THERE ARE 49 CAPLUS RECORDS THAT CITE THIS  
 RECORD (49 CITINGS)

L15 ANSWER 24 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1991:655797 CAPLUS  
 DOCUMENT NUMBER: 115:255797  
 ORIGINAL REFERENCE NO.: 115:43481a, 43484a  
 TITLE: Preparation and use of catechol derivatives as medical  
 antioxidants

INVENTOR(S): Korkolainen, Tapio Juhani; Nissinen, Erkki Aarne  
Olavi; Backstrom, Reijo Johannes; Pippuri, Aino  
Kyllikki  
PATENT ASSIGNEE(S): Orion-Yhtymä Oy, Finland  
SOURCE: Eur. Pat. Appl., 14 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 4  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 444899	A2	19910904	EP 1991-301587	19910227
EP 444899	A3	19921125		
EP 444899	B1	19970205		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 04211627	A	19920803	JP 1991-30908	19910226
JP 3157846	B2	20010416		
AT 148626	T	19970215	AT 1991-301587	19910227
HR 9201250	B1	20000630	HR 1992-1250	19921112
US 5489614	A	19960206	US 1995-461752	19950605
PRIORITY APPLN. INFO.:				
			YU 1989-21	A 19890106
			GB 1990-4348	A 19900227
			FI 1986-4875	A 19861128
			GB 1987-12437	A 19870528
			US 1987-126911	A3 19871127
			US 1988-288979	A2 19881223
			US 1990-587791	A2 19900925
			US 1991-658666	B1 19910221
			US 1994-294762	B1 19940823
OTHER SOURCE(S): MARPAT 115:255797				
GI				



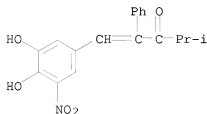
AB The title compds. [I; R2 = CH:CR3R4, CH2CHR3R4; R3 = acyl, cyclopropylcarbonyl; R4 = (un)substituted aryl, cyclopropylcarbonyl; X = halo, NO2, cyano, CF3, CHO, CO2H], their physiol. acceptable salts and esters, are claimed. Also claimed are the use of the known I (R2 = H, substituted alkyl, alkoxy, aryl, heterocyclyl, NO2, cyano, CHO, CO2H, CH:CR3R4, CH2CHR3R4; broader definitions for R3, R4 are given; X as above) and of their physiol. acceptable salts and esters for the prophylaxis and treatment of tissue damage induced in lipid peroxidn., e.g., in heart disease, rheumatoid arthritis, cancer, etc. Thus, a solution of Me2CHCOCH2Ph and 3,4,5-(HO)2(O2N)C6H2CHO in Me2CHOH was saturated by HCl(g) at 20° and stirred 4 h at room temperature to give title compound I (R2 = Me2CHCOCH2Ph:CH, X = O2N). The latter in a controlled peroxidn. test in vitro had a stoichiometric factor 3.3 vs 2.0 for Trolox and 0.7 for ascorbic acid.

IT 137419-33-1P 137419-37-5P 137419-38-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as medical antioxidant)

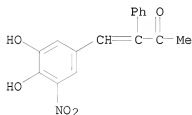
RN 137419-33-1 CAPLUS

CN 1-Penten-3-one, 1-(3,4-dihydroxy-5-nitrophenyl)-4-methyl-2-phenyl- (CA INDEX NAME)



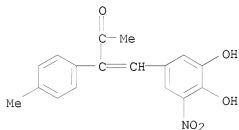
RN 137419-37-5 CAPLUS

CN 3-Buten-2-one, 4-(3,4,4-dihydroxy-5-nitrophenyl)-3-phenyl- (CA INDEX NAME)



RN 137419-38-6 CAPLUS

CN 3-Buten-2-one, 4-(3,4,4-dihydroxy-5-nitrophenyl)-3-(4-methylphenyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
(3 CITINGS)

=> d ibib abs hitstr 15-19

L15 ANSWER 15 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:808259 CAPLUS

DOCUMENT NUMBER: 134:97896

TITLE: Mappain, a new cytotoxic prenylated stilbene from  
Macaranga mappia

AUTHOR(S): van der Kaaden, Jacobus E.; Hemscheidt, Thomas K.;  
Mooberry, Susan L.

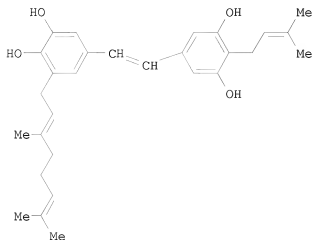
CORPORATE SOURCE: Department of Chemistry, University of Hawaii at  
Manoa, Honolulu, HI, 96822, USA

SOURCE: Journal of Natural Products (2001), 64(1), 103-105



PUBLISHER:  
DOCUMENT TYPE:  
LANGUAGE:  
GI

CODEN: JNPRDF; ISSN: 0163-3864  
American Chemical Society  
Journal  
English



I

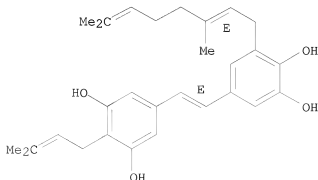
AB A new prenylated stilbene, mappain (I), was isolated from leaves of *Macaranga mappia* by bioassay-guided fractionation. The structure was established by application of spectroscopic methods. Mappain is cytotoxic but it appears to be a poor substrate for P-glycoprotein-mediated transport because it is equally potent and effective against the drug-sensitive SK-OV-3 and drug-resistant SKVLE-1 ovarian cancer cell lines, exhibiting an IC<sub>50</sub> value of 1.3  $\mu$ M in both cases.

IT 319915-14-5P, Mappain  
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
(cytotoxic prenylated stilbene from *Macaranga mappia*)

RN 319915-14-5 CAPLUS

CN 1,2-Benzenediol, 5-[(1E)-2-[3,5-dihydroxy-4-(3-methyl-2-buten-1-yl)phenyl]ethenyl]-3-[(2E)-3,7-dimethyl-2,6-octadien-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD  
(7 CITINGS)  
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 16 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:801085 CAPLUS

DOCUMENT NUMBER: 132:175303

TITLE: Synthesis and Reactivity of a Potential Carcinogenic  
Metabolite of Tamoxifen:

3,4-Dihydroxytamoxifen-o-quinone  
Zhang, Fagen; Fan, Peter W.; Liu, Xuemei; Shen, Lixin;  
Van Breemen, Richard B.; Bolton, Judy L.

CORPORATE SOURCE: Department of Medicinal Chemistry and Pharmacognosy  
(M/C 781) College of Pharmacy, University of Illinois  
at Chicago, Chicago, IL, 60612-7231, USA

SOURCE: Chemical Research in Toxicology (2000), 13(1), 53-62  
CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Although tamoxifen is approved for the treatment of hormone-dependent breast cancer as well as for the prevention of breast cancer in high-risk women, several studies in animal models have shown that tamoxifen is hepatocarcinogenic, and in humans, tamoxifen has been associated with an increased risk of endometrial cancer. One potential mechanism of tamoxifen carcinogenesis could involve metabolism of tamoxifen to 3,4-dihydroxytamoxifen followed by oxidation to a highly reactive o-quinone which has the potential to alkylate and/or oxidize cellular macromols. in vivo. In the study presented here, the authors synthesized the 3,4-dihydroxytamoxifen, prepared its o-quinone chemical and enzymically, and studied the reactivity of the o-quinone with GSH and deoxynucleosides. The E (trans) and Z (cis) isomers of 3,4-dihydroxytamoxifen were synthesized using a concise synthetic pathway (four steps). This approach is based on the McMurtry reaction between the key 4-(2-chloroethoxy)-3,4-methylenedioxybenzophenone and propiophenone, followed by selective removal of the methylenedioxy ring of (E,Z)-1-[4-(2-(N,N-dimethylamino)ethoxy)phenyl]-1-(3,4-methylenedioxyphenyl)-2-phenyl-1-butene with BC13. Oxidation of 3,4-dihydroxytamoxifen by activated silver oxide or tyrosinase gave 3,4-dihydroxytamoxifen-o-quinone as a mixture of E and Z isomers. The resulting o-quinone has a half-life of approx. 80 min under physiol. conditions. Reaction of the o-quinone with GSH gave two di-GSH conjugates and three mono GSH conjugates. Incubation of 3,4-dihydroxytamoxifen with GSH in the presence of microsomal P 450 gave the same GSH conjugates which were also detected in incubations with human breast cancer cells (MCF-7). Reaction of 3,4-dihydroxytamoxifen-o-quinone with deoxynucleosides gave only thymidine and deoxyguanosine adducts; neither deoxyadenosine nor deoxycytosine adducts were detected. Preliminary studies conducted with human breast cancer cell lines showed that 3,4-dihydroxytamoxifen exhibited cytotoxic potency similar to that of 4-hydroxytamoxifen and tamoxifen in an estrogen receptor neg. (ER-) cell line (MDA-MB-231); however, in the ER+ cell line (MCF-7), the catechol metabolite was about half as toxic as the other two compds. Finally, in the presence of microsomes and GSH, 4-hydroxytamoxifen gave predominantly quinone methide GSH conjugates as reported in the previous paper in this issue [Fan, P. W., et al. (2000) Chemical Res. Toxicol. 13, XX-XX]. However, in the presence of tyrosinase and GSH, 4-hydroxytamoxifen was primarily converted to o-quinone GSH conjugates. These results suggest that the catechol metabolite of tamoxifen has the potential to cause cytotoxicity in vivo through formation of 3,4-dihydroxytamoxifen-o-quinone.

IT 65319-40-6P, (Z)-3,4-Dihydroxytamoxifen 81992-84-9P,

(E)-3,4-Dihydroxytamoxifen

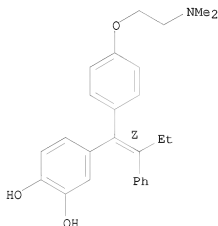
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(synthesis and reactivity of a potential carcinogenic metabolite of tamoxifen dihydroxytamoxifen-o-quinone in relation to breast cancer inhibition)

RN 65319-40-6 CAPLUS

CN 1,2-Benzenediol, 4-[(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

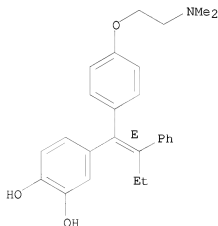
Double bond geometry as shown.



RN 81992-84-9 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



IT 259149-80-9 259149-81-0 259149-82-1

RL: BSU (Biological study, unclassified); FMU (Formation, unclassified); MFU (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)

(synthesis and reactivity of a potential carcinogenic metabolite of

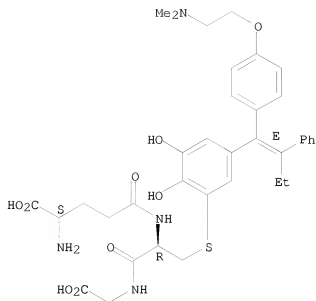
RN 259149-80-9 CAPLUS

Absolute stereochemistry.

RN 259149-81-0 CAPLUS

Absolute stereochemistry.

Double bond geometry as shown.

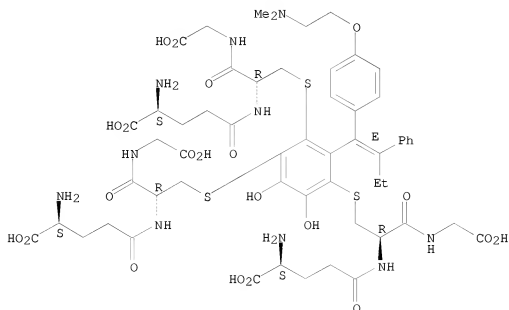


RN 259149-82-1 CAPLUS

CN Glycine, 2,2',2''-[3-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-5,6-dihydroxy-1,2,4-benzenetriyl]tris[L-γ-glutamyl-L-cysteinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

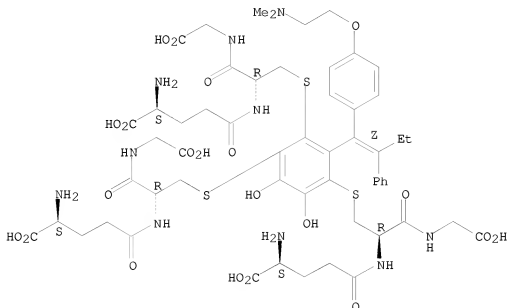


IT 259149-75-2

RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)  
(synthesis and reactivity of a potential carcinogenic metabolite of tamoxifen dihydroxytamoxifen-o-quinone in relation to breast cancer inhibition)

RN 259149-75-2 CAPLUS  
 CN Glycine, 2,2',2''-[3-[(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-5,6-dihydroxy-1,2,4-benzenetriyl]tris[L-γ-glutamyl-L-cysteinyl- (9CI) (CA INDEX NAME)

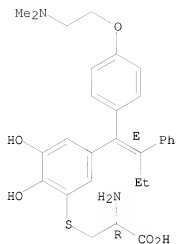
Absolute stereochemistry.  
 Double bond geometry as shown.



IT 259149-73-0 259149-74-1 259149-76-3  
 259149-77-4 259149-78-5 259149-79-6  
 RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)  
 (synthesis and reactivity of a potential carcinogenic metabolite of  
 tamoxifen dihydroxytamoxifen-o-quinone in relation to breast  
 cancer inhibition)

RN 259149-73-0 CAPLUS  
 CN L-Cysteine, S-[5-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]-2,3-dihydroxyphenyl]- (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.

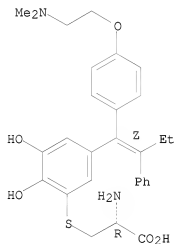


RN 259149-74-1 CAPLUS

CN L-Cysteine, S-[5-[(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]-2,3-dihydroxyphenyl]- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

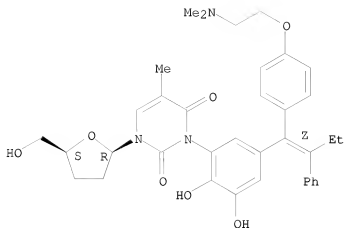


RN 259149-76-3 CAPLUS

CN Thymidine, 3'-deoxy-3-[5-[(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

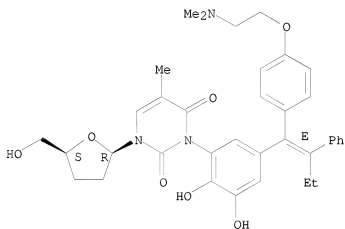


RN 259149-77-4 CAPLUS

CN Thymidine, 3'-deoxy-3-[5-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



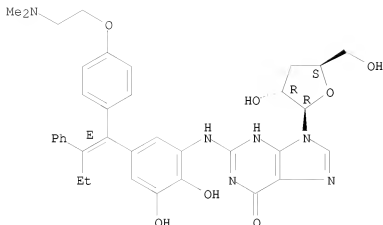
RN 259149-78-5 CAPLUS

CN Guanosine, 3'-deoxy-N-[5-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



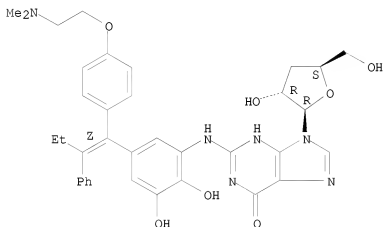


RN 259149-79-6 CAPLUS

CN Guanosine, 3'-deoxy-N-[5-[1(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



OS.CITING REF COUNT: 39 THERE ARE 39 CAPLUS RECORDS THAT CITE THIS RECORD (39 CITINGS)

REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 17 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:796363 CAPLUS

DOCUMENT NUMBER: 132:160795

TITLE: 4-Hydroxylated Metabolites of the Antiestrogens Tamoxifen and Toremifene Are Metabolized to Unusually Stable Quinone Methides

AUTHOR(S): Fan, Peter W.; Zhang, Fagen; Bolton, Judy L.

CORPORATE SOURCE: Department of Medicinal Chemistry and Pharmacognosy (M/C 781) College of Pharmacy, University of Illinois at Chicago, Chicago, IL, 60612-7231, USA

SOURCE: Chemical Research in Toxicology (2000), 13(1), 45-52 CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal  
LANGUAGE: English

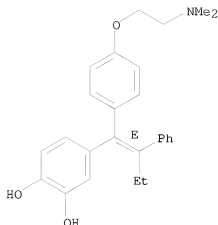
AB Tamoxifen is widely prescribed for the treatment of hormone-dependent breast cancer, and it has recently been approved by the Food and Drug Administration for the chemoprevention of this disease. However, long-term usage of tamoxifen has been linked to increased risk of developing endometrial cancer in women. One of the suggested pathways leading to the potential toxicity of tamoxifen involves its oxidative metabolism to 4-hydroxytamoxifen, which may be further oxidized to an electrophilic quinone methide. The resulting quinone methide has the potential to alkylate DNA and may initiate the carcinogenic process. To further probe the chemical reactivity and toxicity of such an electrophilic species, the authors have prepared the 4-hydroxytamoxifen quinone methide chemical and enzymically, examined its reactivity under physiol. conditions, and quantified its reactivity with GSH. Interestingly, this quinone methide is unusually stable; its half-life under physiol. conditions is approx. 3 h, and its half-life in the presence of GSH is approx. 4 min. The reaction between 4-hydroxytamoxifen quinone methide and GSH appears to be a reversible process because the quinone methide GSH conjugates slowly decompose over time, regenerating the quinone methide as indicated by LC/MS/MS data. The tamoxifen GSH conjugates were detected in microsomal incubations with 4-hydroxytamoxifen; however, none were observed in breast cancer cell lines (MCF-7) perhaps because very little quinone methides is formed. Toremifene, which is a chlorinated analog of tamoxifen, undergoes similar oxidative metabolism to give 4-hydroxytoremifene, which is further oxidized to the corresponding quinone methide. The toremifene quinone methide has a half-life of approx. 1 h under physiol. conditions, and its rate of reaction in the presence of excess GSH is approx. 6 min. More detailed analyses have indicated that the 4-hydroxytoremifene quinone methide reacts with two mols. of GSH and loses chlorine to give the corresponding di-GSH conjugates. The reaction mechanism likely involves an episulfonium ion intermediate which may contribute to the potential cytotoxic effects of toremifene. Similar to what was observed with 4-hydroxytamoxifen, 4-hydroxytoremifene was metabolized to di-GSH conjugates in microsomal incubations at about 3 times the rate of 4-hydroxytamoxifen, although no conjugates were detected with MCF-7 cells. Finally, these data suggest that quinone methide formation may not make a significant contribution to the cytotoxic and genotoxic effects of tamoxifen and toremifene.

IT 81992-84-9, 3,4-Dihydroxytamoxifen  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(hydroxylated metabolites of antiestrogens tamoxifen and toremifene are metabolized to unusually stable quinone methides in relation to conjugate formation with GSH and carcinogenicity)

RN 81992-84-9 CAPLUS

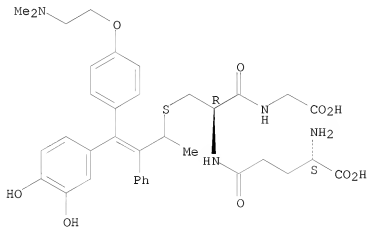
CN 1,2-Benzenediol, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



IT 259087-29-1  
 RL: BSU (Biological study, unclassified); FMU (Formation, unclassified);  
 MFM (Metabolic formation); BIOL (Biological study); FORM (Formation,  
 nonpreparative)  
 (hydroxylated metabolites of antiestrogens tamoxifen and toremifene are  
 metabolized to unusually stable quinone methides in relation to  
 conjugate formation with GSH and carcinogenicity)  
 RN 259087-29-1 CAPLUS  
 CN Glycine, L-γ-glutamyl-S-[3-(3,4-dihydroxyphenyl)-3-[4-[2-  
 (dimethylamino)ethoxy]phenyl]-1-methyl-2-phenyl-2-propenyl]-L-cysteinyl-  
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry unknown.

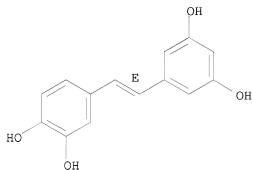


OS.CITING REF COUNT: 50 THERE ARE 50 CAPLUS RECORDS THAT CITE THIS  
 RECORD (52 CITINGS)  
 REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 18 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1999:467829 CAPLUS  
 DOCUMENT NUMBER: 131:266661  
 TITLE: Piceatannol, a stilbene phytochemical, inhibits  
 mitochondrial F0F1-ATPase activity by targeting the F1

complex  
 AUTHOR(S): Zheng, Jianbiao; Ramirez, Victor D.  
 CORPORATE SOURCE: Department of Molecular and Integrative Physiology,  
 University of Illinois at Urbana-Champaign, Urbana,  
 IL, 61801, USA  
 SOURCE: Biochemical and Biophysical Research Communications  
 (1999), 261(2), 499-503  
 CODEN: BBRC99; ISSN: 0006-291X  
 PUBLISHER: Academic Press  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Piceatannol is a stilbene phytochem. from the seeds of Euphorbia lagascae,  
 previously identified as an antileukemic principle. Piceatannol is  
 considered an inhibitor of several tyrosine kinases. We recently reported  
 that resveratrol, another stilbene phytoalexin from grape seeds, was an  
 inhibitor of ATP synthase. Here, we demonstrated that piceatannol  
 potently inhibited the rat brain mitochondrial F0F1-ATPase activity in  
 both solubilized and submitochondrial preps. (IC50 of 8-9  $\mu$ M), while  
 having relatively small effect on the Na<sup>+</sup>, K<sup>+</sup>-ATPase activity of porcine  
 cerebral cortex (no effect up to 7  $\mu$ M). Piceatannol inhibited the  
 ATPase activity of the purified rat liver F1 with IC50 of about 4  $\mu$ M,  
 while resveratrol was slightly less active (IC50 of about 14  $\mu$ M). Our  
 results indicate that piceatannol and resveratrol inhibit the F-type  
 ATPase by targeting the F1 sector, which is located to the inner membrane  
 of mitochondria and plasma membrane of normal endothelial cells and  
 several cancer cell lines. This mechanism could potentially  
 contribute to the multiple effects of these chemopreventive phytochems.  
 (c) 1999 Academic Press.  
 IT 10083-24-6, Piceatannol  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); BIOL (Biological study)  
 (piceatannol inhibits mitochondrial F0F1-ATPase activity by targeting  
 the F1 complex)  
 RN 10083-24-6 CAPLUS  
 CN 1,2-Benzenediol, 4-[(1E)-2-(3,5-dihydroxyphenyl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

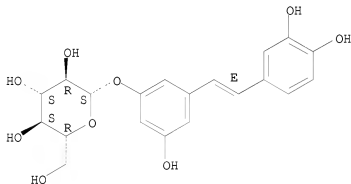


OS.CITING REF COUNT: 55 THERE ARE 55 CAPLUS RECORDS THAT CITE THIS  
 RECORD (55 CITINGS)  
 REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 19 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1999:379085 CAPLUS  
 DOCUMENT NUMBER: 131:169463  
 TITLE: Determination of Stilbenes (trans-Astringin, cis- and  
 trans-Piceid, and cis- and trans-Resveratrol) in

AUTHOR(S): Portuguese Wines  
 Ribeiro de Lima, Maria T.; Waffo-Teguo, Pierre;  
 Teissedre, Pierre L.; Pujolas, Agnes; Vercauteren,  
 Joseph; Cabanis, Jean C.; Merillon, Jean M.  
 CORPORATE SOURCE: Faculte des Sciences Pharmaceutiques Centre de  
 Formation et de Recherche en Enologie, Universite de  
 Montpellier I, Montpellier, 34060, Fr.  
 SOURCE: Journal of Agricultural and Food Chemistry (1999),  
 47(7), 2666-2670  
 CODEN: JAFCAU; ISSN: 0021-8561  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Stilbenes have been shown to have cancer chemopreventive  
 activity and to protect lipoproteins from oxidative damage. A method is  
 described for their direct determination in different types of wine using HPLC  
 with UV detection. In a survey of 120 com. wines from Portugal and  
 France, the highest concns. of stilbenes were found in red wines. The  
 glucosides of resveratrol were present in higher concns. than the free  
 isomers. Isolation from wine and characterization of trans-astringin in a  
 large quantity are described for the 1st time.  
 IT 29884-49-9  
 RL: ANT (Analyte); ANST (Analytical study)  
 (determination of stilbenes in Portuguese wines)  
 RN 29884-49-9 CAPLUS  
 CN  $\beta$ -D-Glucopyranoside, 3-[(1E)-2-(3,4-dihydroxyphenyl)ethenyl]-5-  
 hydroxyphenyl (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



OS.CITING REF COUNT: 32 THERE ARE 32 CAPLUS RECORDS THAT CITE THIS  
 RECORD (32 CITINGS)  
 REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L15 ANSWER 10 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2002:57665 CAPLUS  
 DOCUMENT NUMBER: 137:163396  
 TITLE: Ellagic acid inhibits nucleoside diphosphate kinase-B  
 activity  
 AUTHOR(S): Malmquist, N. A.; Anzinger, J. J.; Hirzel, D.; Buxton,  
 I. L. O.  
 CORPORATE SOURCE: Department of Pharmacology, University of Nevada

SOURCE: School of Medicine, Reno, NV, 89557, USA  
 Proceedings of the Western Pharmacology Society  
 (2001), 44, 57-59  
 CODEN: PWPSA8; ISSN: 0083-8969

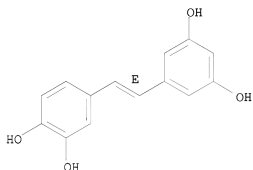
PUBLISHER: Western Pharmacology Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Various compds. that have anti-angiogenesis or general anti-cancer properties, such as polyphenolic tea compds., nucleoside analogs AZT, PAPS, and 8-Cl-cAMP, and ellagic acid, were examined for their ability to inhibit nucleoside diphosphate kinase-B (NDPK-B) activity. NDPK-B activity was inhibited by the polyphenolic constituents of tea, i.e., EGCG, ECG and theaflavins. The nucleoside analogs, 8-Cl-cAMP and PAPS, inhibited NDPK-B transphosphorylation activity at relatively low potency. Ellagic acid (hexahydroxydiphenic acid dilactone), found through a structure search based on the conserved moiety contained in the most potent NDPK-B inhibiting polyphenolic tea compds., had the highest affinity of NDPK-B.

IT 10083-24-6, Piceatannol  
 RL: PAC (Pharmacological activity); BIOL (Biological study)  
 (effects of tea polyphenols and nucleoside analogs on nucleoside diphosphate kinase-B activity)

RN 10083-24-6 CAPLUS  
 CN 1,2-Benzenediol, 4-[(1E)-2-(3,5-dihydroxyphenyl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 11 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2001:855006 CAPLUS  
 DOCUMENT NUMBER: 136:128734  
 TITLE: Synthesis and Reactivity of Potential Toxic Metabolites of Tamoxifen Analogues: Droloxifene and Toremifene o-Quinones

AUTHOR(S): Yao, Dan; Zhang, Fagen; Yu, Linning; Yang, Yanan; van Breemen, Richard B.; Bolton, Judy L.

CORPORATE SOURCE: Department of Medicinal Chemistry and Pharmacognosy (M/C 781) College of Pharmacy, University of Illinois at Chicago, Chicago, IL, 60612-7231, USA

SOURCE: Chemical Research in Toxicology (2001), 14(12), 1643-1653  
 CODEN: CRTOEC; ISSN: 0893-228X

PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal

LANGUAGE: English

AB Tamoxifen remains the endocrine therapy of choice in the treatment of all stages of hormone-dependent breast cancer. However, tamoxifen has been shown to increase the risk of endometrial cancer which has stimulated research for new effective antiestrogens, such as droloxifene and toremifene. In this study, the potential for these compds. to cause cytotoxic effects was investigated. One potential cytotoxic mechanism could involve metabolism of droloxifene and toremifene to catechols, followed by oxidation to reactive o-quinones. Another cytotoxic pathway could involve the oxidation of 4-hydroxytoremifene to an electrophilic quinone methide. Comparison of the amts. of GSH conjugates formed from 4-hydroxytamoxifen, droloxifene, and 4-hydroxytoremifene suggested that 4-hydroxytoremifene is more effective at formation of a quinone methide. However, all three substrates formed similar amts. of o-quinones. Both the tamoxifen-o-quinone and toremifene-o-quinone reacted with deoxynucleosides to give corresponding adducts. However, the toremifene-o-quinone was shown to be considerably more reactive than the tamoxifen-o-quinone in terms of both kinetic data as well as the yield and type of deoxynucleoside adducts formed. Since thymidine formed the most abundant adducts with the toremifene-o-quinone, sufficient material was obtained for characterization by 1H NMR, COSY-NMR, DEPT-NMR, and tandem mass spectrometry. Cytotoxicity studies with tamoxifen, droloxifene, 4-hydroxytamoxifen, 4-hydroxytoremifene, and their catechol metabolites were carried out in the human breast cancer cell lines S30 and MDA-MB-231. All of the metabolites tested showed cytotoxic effects that were similar to the parent antiestrogens which suggests that o-quinone formation from tamoxifen, droloxifene, and 4-hydroxytoremifene is unlikely to contribute to their cytotoxicity. However, the fact that the o-quinones formed adducts with deoxynucleosides in vitro implies that the o-quinone pathway might contribute to the genotoxicity of the antiestrogens in vivo.

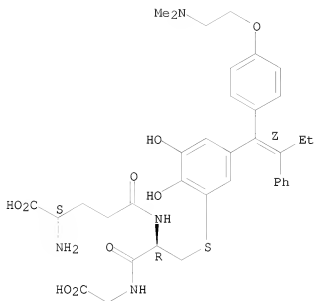
IT 259149-80-9 259149-81-0 392710-66-6  
392725-33-6 392725-34-7 392725-35-8  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(synthesis and reactivity of toxic metabolites of tamoxifen analogs,  
droloxifene and toremifene o-quinones)

RN 259149-80-9 CAPLUS

CN Glycine, L-γ-glutamyl-S-[5-[(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]-L-cysteiny- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

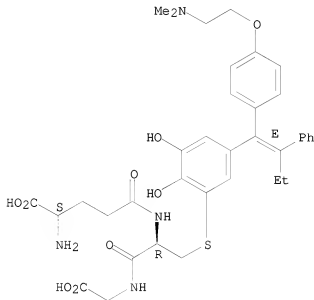
Double bond geometry as shown.



RN 259149-81-0 CAPLUS

CN Glycine, L-γ-glutamyl-S-[5-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

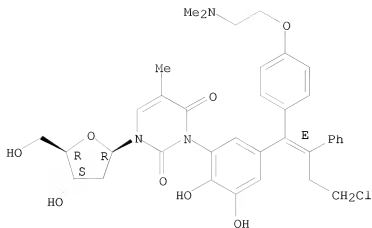


RN 392710-66-6 CAPLUS

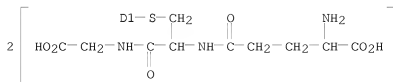
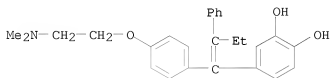
CN Thymidine, 3-[5-[(1E)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

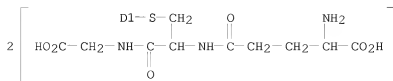
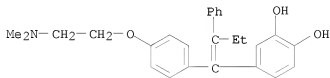




RN 392725-33-6 CAPLUS  
 CN Glycine, 2,2'-[[ (1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]dihydroxyphenylene]bis[L-γ-glutamyl-L-cysteiny]- (9CI) (CA INDEX NAME)

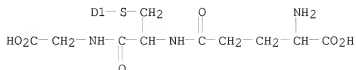
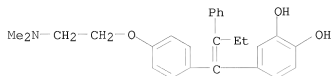


RN 392725-34-7 CAPLUS  
 CN Glycine, 2,2'-[[ (1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]dihydroxyphenylene]bis[L-γ-glutamyl-L-cysteiny]- (9CI) (CA INDEX NAME)



RN 392725-35-8 CAPLUS

CN Glycine, L- $\gamma$ -glutamyl-S-[[1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]dihydroxyphenyl]-L-cysteinyl- (9CI) (CA INDEX NAME)



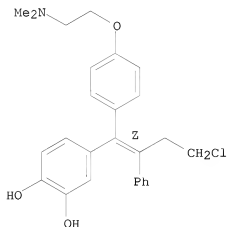
IT 392710-51-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(synthesis and reactivity of toxic metabolites of tamoxifen analogs, droloxifene and toremifene o-quinones)

RN 392710-51-9 CAPLUS

CN 1,2-Benzenediol, 4-[(1Z)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



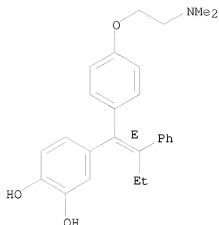
IT 81992-84-9, 3,4-Dihydroxytamoxifen

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(synthesis and reactivity of toxic metabolites of tamoxifen analogs, droloxifene and toremifene o-quinones)

RN 81992-84-9 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



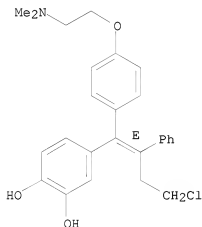
IT 392710-49-5P 392710-55-3P 392710-57-5P  
 392710-58-6P 392710-60-0P 392710-61-1P  
 392725-30-3P 392725-31-4P 392725-32-5P  
 392725-36-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis and reactivity of toxic metabolites of tamoxifen analogs,  
 droloxifene and toremifene o-quinones)

RN 392710-49-5 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

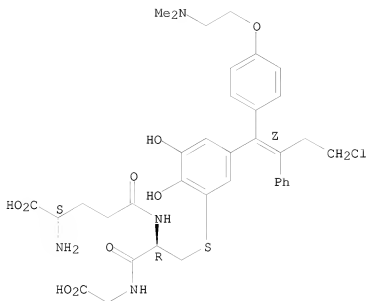


RN 392710-55-3 CAPLUS

CN Glycine, L-γ-glutamyl-S-[5-[(1Z)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

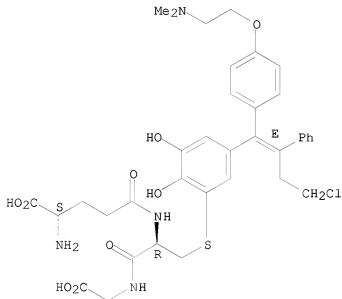
Double bond geometry as shown.



RN 392710-57-5 CAPLUS

CN Glycine, L- $\gamma$ -glutamyl-S-[5-[(1E)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

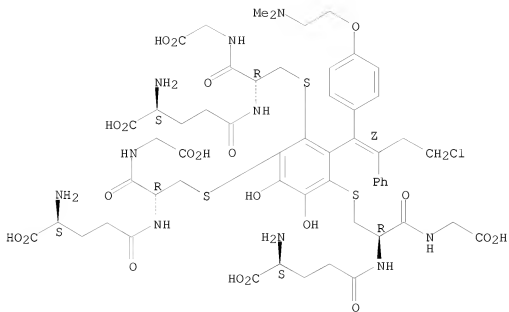
Absolute stereochemistry.  
Double bond geometry as shown.



RN 392710-58-6 CAPLUS

CN Glycine, 2,2',2'''-[3-[(1Z)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-5,6-dihydroxy-1,2,4-benzenetriyl]tris[L- $\gamma$ -glutamyl-L-cysteinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

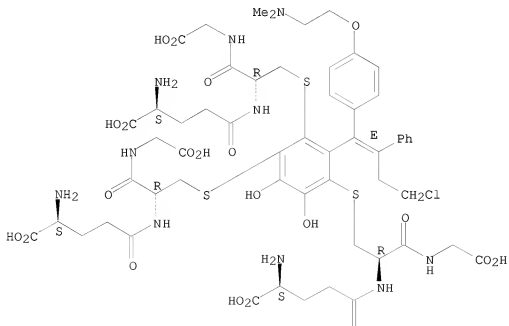


RN 392710-60-0 CAPLUS

CN Glycine, 2,2',2''-[3-[(1E)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-5,6-dihydroxy-1,2,4-benzenetriyl]tris[L-γ-glutamyl-L-cysteinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

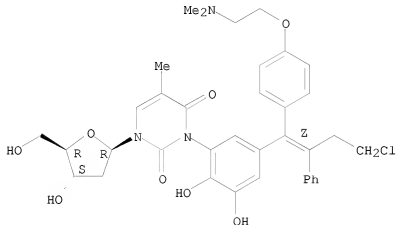
PAGE 1-A



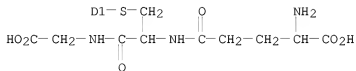
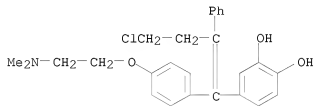


RN 392710-61-1 CAPLUS  
 CN Thymidine, 3-[5-[(1Z)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]-2,3-dihydroxyphenyl]- (9CI) (CA INDEX NAME)

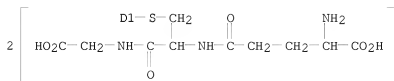
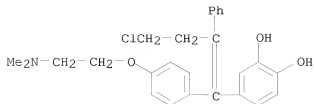
Absolute stereochemistry.  
 Double bond geometry as shown.



RN 392725-30-3 CAPLUS  
 CN Glycine, L-γ-glutamyl-S-[[4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]dihydroxyphenyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

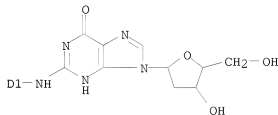
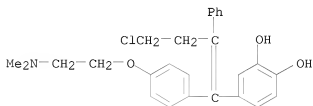


RN 392725-31-4 CAPLUS  
 CN Glycine, 2,2'-[[[(1Z)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]dihydroxyphenylene]bis[L-γ-glutamyl-L-cysteinyl- (9CI) (CA INDEX NAME)



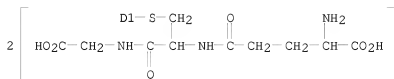
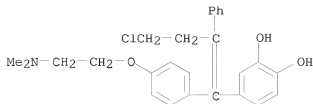
RN 392725-32-5 CAPLUS

CN Guanosine, N-[(1Z)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]dihydroxyphenyl]-2'-deoxy- (9CI) (CA INDEX NAME)



RN 392725-36-9 CAPLUS

CN Glycine, 2,2'-[[(1E)-4-chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-butenyl]dihydroxyphenylene]bis[L-γ-glutamyl-L-cysteinyl- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS  
RECORD (14 CITINGS)  
REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 12 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:657229 CAPLUS

DOCUMENT NUMBER: 136:14976

TITLE: Biomonitoring of urinary tamoxifen and its metabolites from breast cancer patients using nonaqueous capillary electrophoresis with electrospray mass spectrometry

AUTHOR(S): Carter, Spencer J.; Li, Xing-Fang; Mackey, John R.; Modi, Shanu; Hanson, John; Dovichi, Norman J.  
CORPORATE SOURCE: Department of Chemistry, University of Alberta, Edmonton, AB, Can.

SOURCE: Electrophoresis (2001), 22(13), 2730-2736  
CODEN: ELCTDN; ISSN: 0173-0835

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Tamoxifen is an antiestrogen drug used to treat breast cancer. We have extracted tamoxifen and several of its metabolites from urine of patients with both metastatic (stage IV) and locally confined (stages I, II, and III) breast cancer. Anal. of these metabolites was performed by nonaq. capillary electrophoresis with electrospray-mass spectrometry. Peak heights from extracted ion current electropherograms of the metabolites were used to establish a metabolic profile for each patient. We demonstrate substantial variation among patient profiles, statistically significant differences in the amount of urinary tamoxifen N-oxide found in stages I, II, and III compared to stage IV breast cancer patients, and statistically significant differences in the amount of 3,4-dihydroxytamoxifen found in progressors compared to nonprogressors with metastatic (stage IV) cancer.

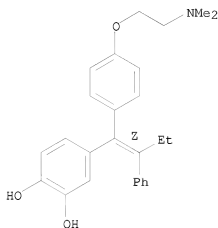
IT 65319-40-6, (Z)-3,4-Dihydroxytamoxifen  
RL: PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(urinary tamoxifen and its metabolites from breast cancer patients)

RN 65319-40-6 CAPLUS

CN 1,2-Benzenediol, 4-[(1Z)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]- (CA INDEX NAME)



Double bond geometry as shown.



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS  
RECORD (19 CITINGS)  
REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 13 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:242398 CAPLUS

DOCUMENT NUMBER: 135:116418

TITLE: Analysis of tamoxifen and its metabolites in synthetic  
gastric fluid digests and urine samples using  
high-performance liquid chromatography with  
electrospray mass spectrometry

AUTHOR(S): Li, X.-F.; Carter, S.; Dovichi, N. J.; Zhao, J. Y.;  
Kovarik, P.; Sakuma, T.

CORPORATE SOURCE: University of Alberta, Edmonton, AB, T6G 2G2, Can.  
SOURCE: Journal of Chromatography, A (2001), 914(1-2), 5-12

CODEN: JCRAEY; ISSN: 0021-9673

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors report on the transformation of tamoxifen at 37° in  
synthetic gastric fluid as studied by HPLC with triple quadrupole mass  
spectrometry. The major transformation products detected were (E)-isomer  
of tamoxifen, metabolite D, and several unidentified components having m/z  
404. Addition of pepsin to the gastric fluid inhibited formation of all of  
these products. The authors analyzed several urine samples from breast  
cancer patients undergoing tamoxifen treatment. Metabolite D was  
identified in the urine samples and in the gastric fluid digest at a  
retention time of 22.0 min eluting from a reversed-phase HPLC column.  
Although several metabolites were found in all the urine samples of  
patients, some metabolites were detected in one sample but not others,  
suggesting tamoxifen metabolism varies in patients.

IT 81992-84-9

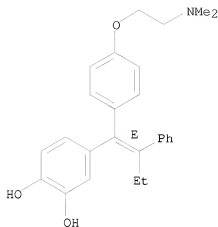
RL: ANT (Analyte); ANST (Analytical study)

(anal. of tamoxifen and its metabolites in synthetic gastric fluid  
digests and urine samples using high-performance liquid chromatog. with  
electrospray mass spectrometry)

RN 81992-84-9 CAPLUS

CN 1,2-Benzenediol, 4-[(1E)-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-  
buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD  
(2 CITINGS)  
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 14 OF 26 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:828028 CAPLUS

DOCUMENT NUMBER: 134:127813

TITLE: Substrate Competitive Inhibitors of IGF-1 Receptor Kinase

AUTHOR(S): Blum, Galia; Gazit, Aviv; Levitzki, Alexander

CORPORATE SOURCE: Department of Biological Chemistry, Alexander  
Silberman Institute of Life Sciences Department of  
Organic Chemistry, Institute of Chemistry The Hebrew  
University of Jerusalem, Jerusalem, 91904, Israel

SOURCE: Biochemistry (2000), 39(51), 15705-15712

CODEN: BICHAW; ISSN: 0006-2960

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

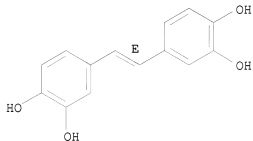
AB IGF-1 and its receptor play a pivotal role in many cancers, and therefore, IGF-1R is an attractive target for the design of inhibitors. In this communication, we report on a number of lead compds. for inhibitors of the isolated IGF-1R kinase. The search for these compds. utilized two novel in vitro assays and was aided by the knowledge of the three-dimensional structure of the insulin receptor kinase domain, which is 84% homologous to the IGF-1R kinase domain. The most potent inhibitor found in these assays was tyrphostin AG 538, with an IC50 = 400 nM. In computer modeling, AG 538 was placed in the kinase domain of the insulin receptor and was able to sit in place of tyrosines 1158 and 1162, which undergo autophosphorylation. Exptl. it is indeed found that AG 538 does not compete with ATP but competes with the IGF-1R substrate. We prepared I-OMe AG 538, which is more hydrophobic and less sensitive to oxidation than AG 538. Both AG 538 and I-OMe AG 538 inhibit IGF-1R autophosphorylation in intact cells in a dose-dependent manner but I-OMe AG 538 is superior, probably because of its enhanced hydrophobic nature. Both compds. inhibit the activation of the downstream targets PKB and Erk2. These findings suggest that AG 538 and I-OMe AG 538 can serve as a lead compound for the development of substrate competitive inhibitors of the IGF-1R. The possible advantage of substrate competitive inhibitors vis-a-vis ATP competitive inhibitors is discussed.

IT 136273-05-7, AG 1233

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

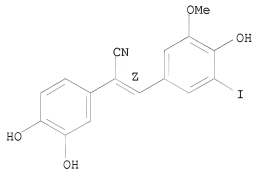
study, unclassified); BIOL (Biological study)  
(substrate competitive inhibitors of IGF-1 receptor kinase)  
RN 136273-05-7 CAPLUS  
CN 1,2-Benzenediol, 4,4'-(1E)-1,2-ethenediylbis- (CA INDEX NAME)

Double bond geometry as shown.



IT 321919-11-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(substrate competitive inhibitors of IGF-1 receptor kinase)  
RN 321919-11-3 CAPLUS  
CN Benzeneacetonitrile, 3,4-dihydroxy- $\alpha$ -[(4-hydroxy-3-iodo-5-methoxyphenyl)methylene]-, ( $\alpha$ Z)- (CA INDEX NAME)

Double bond geometry as shown.



OS.CITING REF COUNT: 89 THERE ARE 89 CAPLUS RECORDS THAT CITE THIS  
RECORD (89 CITINGS)  
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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SINCE FILE	TOTAL
ENTRY	SESSION
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ENTRY	SESSION
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FULL ESTIMATED COST	ENTRY	SESSION
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION
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L16 1 321919-11-3/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND  
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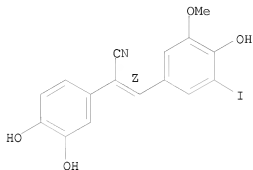
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THE ESTIMATED COST FOR THIS REQUEST IS 6.85 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L16 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2009 ACS on STN  
RN 321919-11-3 REGISTRY  
CN Benzeneacetonitrile, 3,4-dihydroxy- $\alpha$ -[(4-hydroxy-3-iodo-5-methoxyphenyl)methylene]-, ( $\alpha$ Z)- (CA INDEX NAME)  
FS STEREOSEARCH  
MF C16 H12 I N O4  
SR CA  
LC STN Files: CA, CAPLUS  
DT.CA Caplus document type: Journal

RLNP Roles from non-patents: PREP (Preparation)

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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NOTICE SET TO OFF FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

=>

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	4.45	611.07
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-27.88

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provided by InfoChem.

STRUCTURE FILE UPDATES: 27 JUL 2009 HIGHEST RN 1169753-75-6  
DICTIONARY FILE UPDATES: 27 JUL 2009 HIGHEST RN 1169753-75-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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conducting SmartSELECT searches.

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predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information

on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=> s ag 538  
104312 AG  
152 AGS  
104457 AG  
(AG OR AGS)  
11188 538  
L17 3 AG 538  
(AG(W)538)

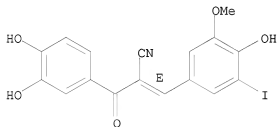
=> d tot

L17 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2009 ACS on STN  
RN 1094048-77-7 REGISTRY  
ED Entered STN: 16 Jan 2009  
CN Benzenepropanenitrile, 3,4-dihydroxy- $\alpha$ -[(4-hydroxy-3-iodo-5-methoxyphenyl)methylene]- $\beta$ -oxo-, ( $\alpha E$ )- (CA INDEX NAME)

OTHER NAMES:

CN I-Me-tyrphostin AG 538  
FS STEREOSEARCH  
MF C17 H12 I N O5  
SR CA  
LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER

Double bond geometry as shown.



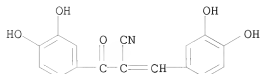
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L17 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2009 ACS on STN  
RN 875283-46-8 REGISTRY  
ED Entered STN: 27 Feb 2006  
CN Benzenepropanenitrile,  $\alpha$ -[(3,4-dihydroxyphenyl)methylene]-3,4-dihydroxy- $\beta$ -oxo- (CA INDEX NAME)

OTHER NAMES:

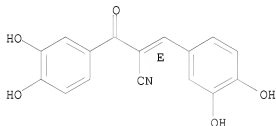
CN Tyrphostin AG 538  
MF C16 H11 N O5  
SR CA  
LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL



5 REFERENCES IN FILE CA (1907 TO DATE)  
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L17 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2009 ACS on STN  
RN 133550-18-2 REGISTRY  
ED Entered STN: 03 May 1991  
CN Benzenepropanenitrile,  $\alpha$ -[(3,4-dihydroxyphenyl)methylene]-3,4-dihydroxy- $\beta$ -oxo-, ( $\alpha$ E)- (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Benzenepropanenitrile,  $\alpha$ -[(3,4-dihydroxyphenyl)methylene]-3,4-dihydroxy- $\beta$ -oxo-, (E)-  
OTHER NAMES:  
CN AG 538  
FS STEREOSEARCH  
MF C16 H11 N O5  
CI COM  
SR CA  
LC STN Files: BEILSTEIN\*, BIOSIS, CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM, TOXCENTER, USPATFULL  
(\*File contains numerically searchable property data)

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

24 REFERENCES IN FILE CA (1907 TO DATE)  
24 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil cap		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	17.33	628.40
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-27.88

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FILE COVERS 1907 - 29 Jul 2009 VOL 151 ISS 5  
FILE LAST UPDATED: 28 Jul 2009 (20090728/ED)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/CAPLUS family of databases have been updated to include new citing references information. This enhancement may impact record import into database management software. For additional information, refer to NEWS 22.

=> s l16

L18 1 L16

=> d

L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2009 ACS on STN  
AN 2000:828028 CAPLUS  
DN 134:127813  
TI Substrate Competitive Inhibitors of IGF-1 Receptor Kinase  
AU Blum, Galia; Gazit, Aviv; Levitzki, Alexander  
CS Department of Biological Chemistry, Alexander Silberman Institute of Life Sciences Department of Organic Chemistry, Institute of Chemistry The Hebrew University of Jerusalem, Jerusalem, 91904, Israel  
SO Biochemistry (2000), 39(51), 15705-15712  
CODEN: BICHAW; ISSN: 0006-2960  
PB American Chemical Society  
DT Journal  
LA English  
OSC.G 89 THERE ARE 89 CAPLUS RECORDS THAT CITE THIS RECORD (89 CITINGS)  
RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> FIL REGISTRY

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

4.25	632.65
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
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CA SUBSCRIBER PRICE

ENTRY      SESSION  
0.00      -27.88

FILE 'REGISTRY' ENTERED AT 10:36:47 ON 29 JUL 2009  
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STRUCTURE FILE UPDATES: 27 JUL 2009 HIGHEST RN 1169753-75-6  
DICTIONARY FILE UPDATES: 27 JUL 2009 HIGHEST RN 1169753-75-6

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conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

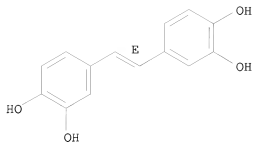
<http://www.cas.org/support/stngen/stdoc/properties.html>

```
=> s ag 1233
      104312 AG
      152 AGS
      104457 AG
              (AG OR AGS)
      3279 1233
L19      1 AG 1233
              (AG(W)1233)
```

=> d

```
L19 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2009 ACS on STN
RN 136273-05-7 REGISTRY
ED Entered STN: 20 Sep 1991
CN 1,2-Benzenediol, 4,4'-(1E)-1,2-ethenediylbis- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2-Benzenediol, 4,4'-(1,2-ethenediyl)bis-, (E)-
OTHER NAMES:
CN AG 1233
FS STEREOSEARCH
MF C14 H12 O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER
```

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

11 REFERENCES IN FILE CA (1907 TO DATE)  
11 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=>

Connection closed by remote host